

11/05/2006 10530136d.trn



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PASSWORD:

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NEWS 3 AUG 09 INSPEC enhanced with 1898-1968 archive  
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NEWS 6 SEP 11 CA/Caplus enhanced with more pre-1907 records  
NEWS 7 SEP 21 CA/Caplus fields enhanced with simultaneous left and right  
truncation  
NEWS 8 SEP 25 CA(SM)/Caplus(SM) display of CA Lexicon enhanced  
NEWS 9 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates  
NEWS 10 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine  
NEWS 11 SEP 28 CEABA-VTB classification code fields reloaded with new  
classification scheme  
NEWS 12 OCT 19 LOGOFF HOLD duration extended to 120 minutes  
NEWS 13 OCT 19 E-mail format enhanced  
NEWS 14 OCT 23 Option to turn off MARPAT highlighting enhancements available  
NEWS 15 OCT 23 CAS Registry Number crossover limit increased to 300,000 in  
multiple databases  
NEWS 16 OCT 23 The Derwent World Patents Index suite of databases on STN  
has been enhanced and reloaded  
NEWS 17 OCT 30 CHEMLIST enhanced with new search and display field  
NEWS 18 NOV 03 JAPIO enhanced with IPC 8 features and functionality  
  
NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8  
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that  
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11/05/2006 10530136d.trn

FILE 'HOME' ENTERED AT 14:51:44 ON 05 NOV 2006

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.21             | 0.21          |

FILE 'REGISTRY' ENTERED AT 14:51:59 ON 05 NOV 2006

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STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4  
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

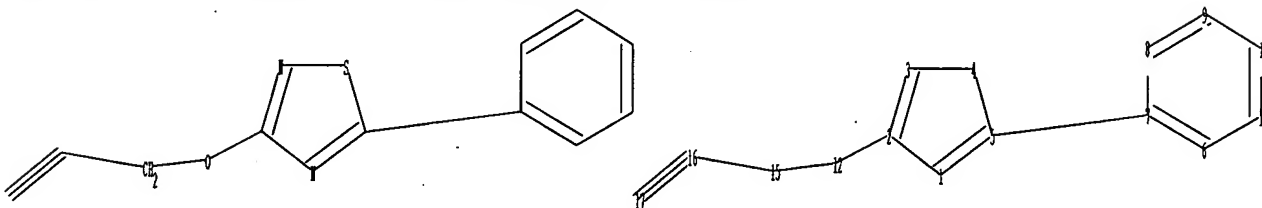
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10530136d.str



chain nodes :

12 15 16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

11/05/2006 10530136d.trn

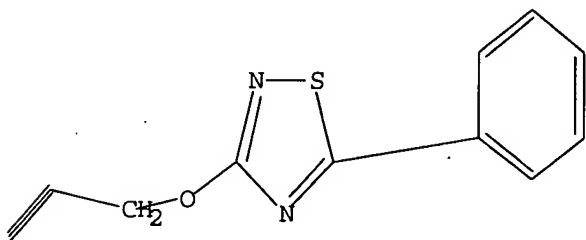
chain bonds :  
2-12 5-7 12-15 15-16 16-17  
ring bonds :  
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11  
exact/norm bonds :  
1-2 1-5 2-3 2-12 3-4  
exact bonds :  
4-5 5-7 12-15 15-16 16-17  
normalized bonds :  
6-7 6-11 7-8 8-9 9-10 10-11  
isolated ring systems :  
containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:CLASS 15:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



G1 O,S,CH2,NH,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
SAMPLE SEARCH INITIATED 14:52:12 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 4 TO 200  
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 sss full

11/05/2006 10530136d.trn

FULL SEARCH INITIATED 14:52:18 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 70 TO ITERATE

100.0% PROCESSED 70 ITERATIONS  
SEARCH TIME: 00.00.01

22 ANSWERS

L3 22 SEA SSS FUL L1

=> FIL HCAPLUS  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| 166.94     | 167.15  |

FILE 'HCAPLUS' ENTERED AT 14:52:21 ON 05 NOV 2006  
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FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20  
FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3  
L4

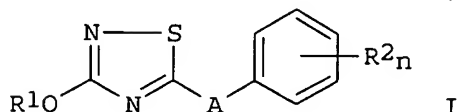
=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:900807 HCAPLUS  
DOCUMENT NUMBER: 137:381259  
TITLE: Preparation of 1,2,4-thiadiazole compounds and arthropodicides containing them  
INVENTOR(S): Ihara, Hideki; Sakamoto, Noriyasu  
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.    | KIND | DATE     | APPLICATION NO. | DATE     |
|---------------|------|----------|-----------------|----------|
| JP 2002338557 | A2   | 20021125 | JP 2001-152269  | 20010522 |

WO 2004041798 A1 20040521 WO 2002-JP11644 20021108  
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
AU 2002368330 A1 20040607 AU 2002-368330 20021108  
BR 2002015911 A 20050726 BR 2002-15911 20021108  
EP 1574505 A1 20050914 EP 2002-808100 20021108  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK  
CN 1688559 A 20051026 CN 2002-829792 20021108  
US 2006167266 A1 20060727 US 2005-530136 20050404  
PRIORITY APPLN. INFO.: JP 2001-152269 A 20010522  
WO 2002-JP11644 A 20021108  
OTHER SOURCE(S): MARPAT 137:381259  
GI



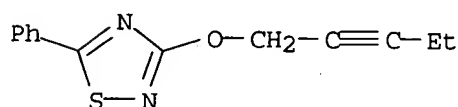
AB The compds. I [R1 = C3-7 (halo)alkenyl; R2 = halo, C1-4 alkyl, C1-3 haloalkyl, C1-4 haloalkoxy, cyano, NO2; n = 0-5; A = O, S, direct bond, CR3R4, NR5; R3, R4 = H, C1-4 alkyl; R5 = H, C1-7 alkyl, C1-3 haloalkyl, C2-4 (halo)alkoxyalkyl, C3-6 (halo)alkenyl, C3-7 (halo)alkynyl, CH2CN] and arthropod control agents containing I are claimed. A composition containing 5-phenyl-3-propargyloxy-1,2,4-thiadiazole (preparation given), showed ≥90% control against Aphis gossypii parasitic on cucumber seedlings.

IT 476315-98-7 476315-99-8 476316-00-4  
476316-01-5 476316-02-6 476316-03-7  
476316-04-8 476316-05-9 476316-06-0  
476316-07-1 476316-08-2 476316-09-3  
476316-10-6 476316-11-7 476316-12-8  
476316-13-9 476316-74-2

RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)  
(preparation of 1,2,4-thiadiazole compds. as arthropodicides)

RN 476315-98-7 HCAPLUS

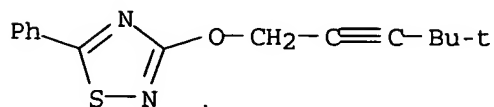
CN 1,2,4-Thiadiazole, 3-(2-pentynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)



RN 476315-99-8 HCAPLUS

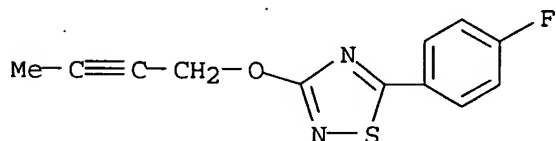
11/05/2006 10530136d.trn

CN 1,2,4-Thiadiazole, 3-[(4,4-dimethyl-2-pentynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



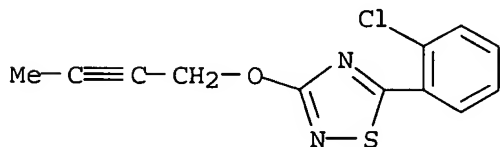
RN 476316-00-4 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



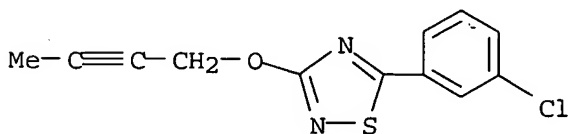
RN 476316-01-5 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



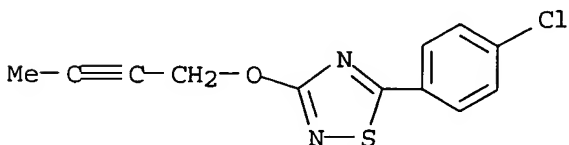
RN 476316-02-6 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 476316-03-7 HCAPLUS

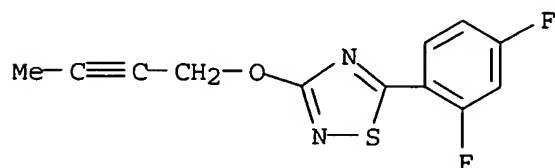
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 476316-04-8 HCAPLUS

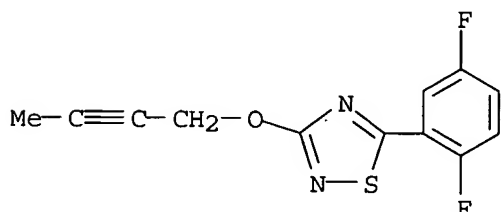
11/05/2006 10530136d.trn

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)



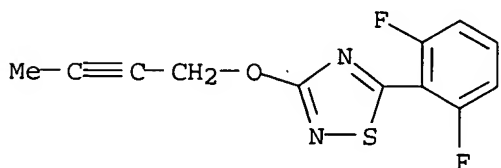
RN 476316-05-9 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,5-difluorophenyl)- (9CI) (CA INDEX NAME)



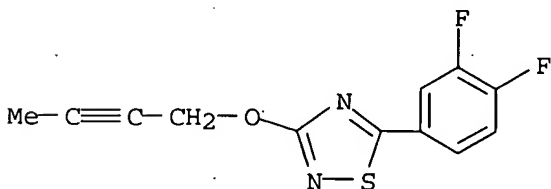
RN 476316-06-0 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,6-difluorophenyl)- (9CI) (CA INDEX NAME)



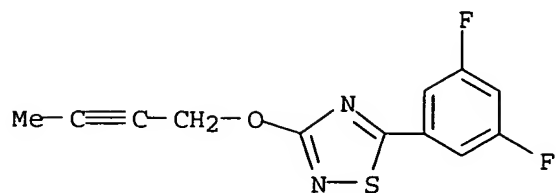
RN 476316-07-1 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,4-difluorophenyl)- (9CI) (CA INDEX NAME)

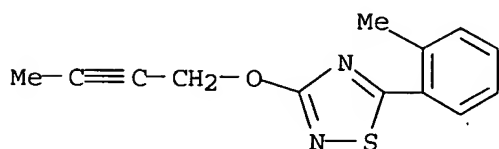


RN 476316-08-2 HCAPLUS

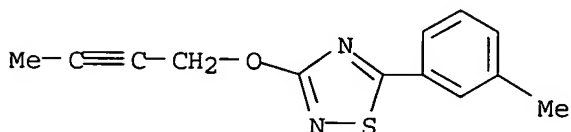
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,5-difluorophenyl)- (9CI) (CA INDEX NAME)



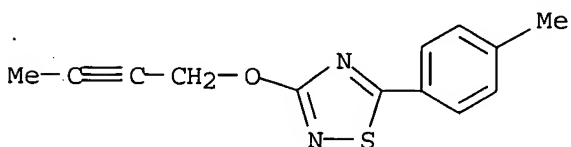
RN 476316-09-3 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)



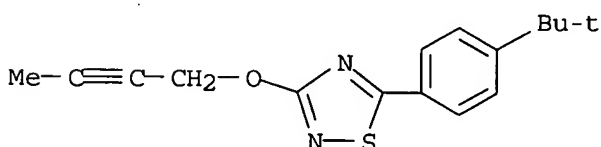
RN 476316-10-6 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-methylphenyl)- (9CI) (CA INDEX NAME)



RN 476316-11-7 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



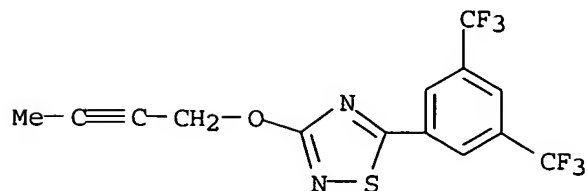
RN 476316-12-8 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 476316-13-9 HCAPLUS  
 CN 1,2,4-Thiadiazole, 5-[3,5-bis(trifluoromethyl)phenyl]-3-(2-butynyloxy)-

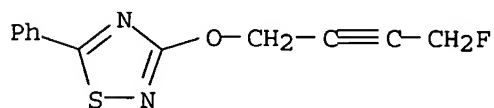


(9CI) (CA INDEX NAME)



RN 476316-74-2 HCAPLUS

CN 1,2,4-Thiadiazole, 3-[(4-fluoro-2-butynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



IT 476315-86-3P 476315-87-4P 476315-89-6P

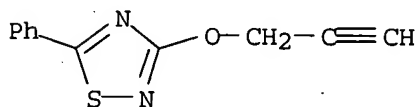
476315-92-1P 476315-94-3P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1,2,4-thiadiazole compds. as arthropodicides)

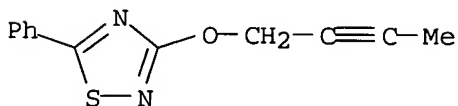
RN 476315-86-3 HCAPLUS

CN 1,2,4-Thiadiazole, 5-phenyl-3-(2-propynyloxy)- (9CI) (CA INDEX NAME)



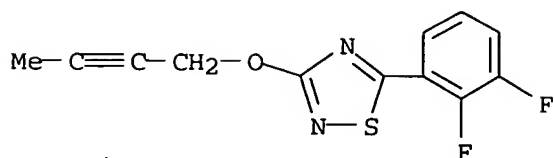
RN 476315-87-4 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)

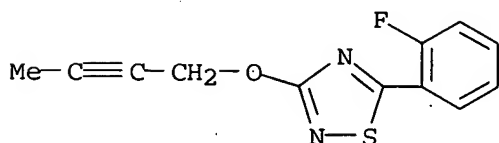


RN 476315-89-6 HCAPLUS

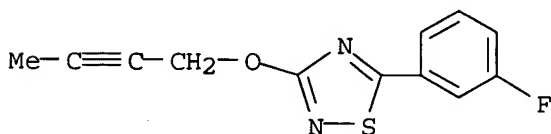
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,3-difluorophenyl)- (9CI) (CA INDEX NAME)



RN 476315-92-1 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 476315-94-3 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-fluorophenyl)- (9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 7.64             | 174.79        |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| -0.75            | -0.75         |

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 14:52:38 ON 05 NOV 2006

11/05/2006 10530136.trn

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

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NEWS 11 SEP 28 CEABA-VTB classification code fields reloaded with new  
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NEWS 14 OCT 23 Option to turn off MARPAT highlighting enhancements available  
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NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.  
  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

11/05/2006 10530136.trn

FILE 'HOME' ENTERED AT 08:33:21 ON 05 NOV 2006

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

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=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.21             | 0.21          |

FILE 'REGISTRY' ENTERED AT 08:33:34 ON 05 NOV 2006

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STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4  
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

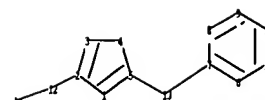
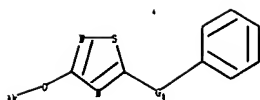
<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10530136.str

11/05/2006

10530136.trn



chain nodes :

12 13 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

2-12 5-13 7-13 12-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 2-3 2-12 3-4 5-13 7-13 12-16

exact bonds :

4-5

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :

containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

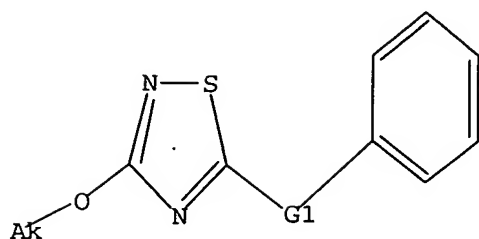
11:Atom 12:CLASS 13:CLASS 16:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 O,S,CH2,NH,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 08:33:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 99 TO ITERATE

100.0% PROCESSED 99 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1384 TO 2576

PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:33:55 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1861 TO ITERATE

100.0% PROCESSED 1861 ITERATIONS

59 ANSWERS

SEARCH TIME: 00.00.01

L3 59 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'HCAPLUS' ENTERED AT 08:34:02 ON 05 NOV 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20

FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

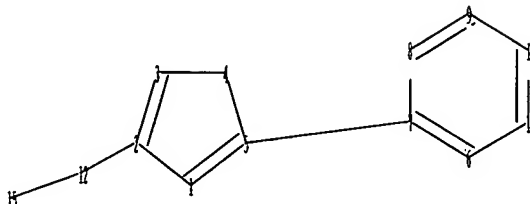
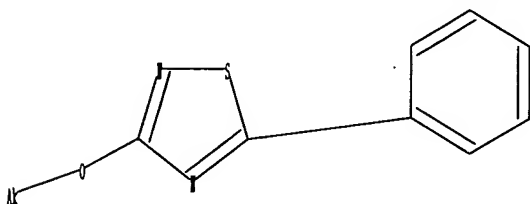
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 13 L3

=>

Uploading C:\Program Files\Stnexp\Queries\10530136a.str



chain nodes :

12 15

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

2-12 5-7 12-15

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 2-3 2-12 3-4 12-15

exact bonds :

4-5 5-7

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :

containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:CLASS 15:CLASS

L5 STRUCTURE UPLOADED

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

5.06

172.21

FILE 'REGISTRY' ENTERED AT 08:35:05 ON 05 NOV 2006

11/05/2006 10530136.trn

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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4  
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

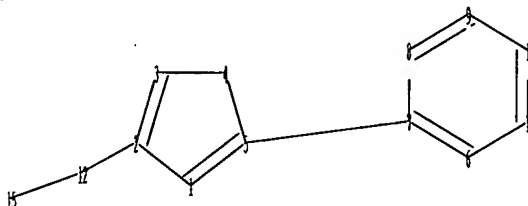
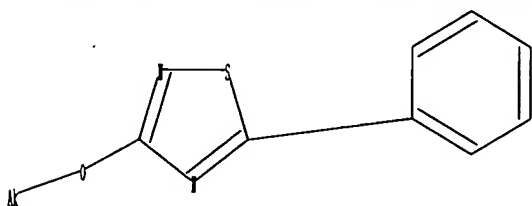
Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10530136a.str



chain nodes :

12 15

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

2-12 5-7 12-15

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 2-3 2-12 3-4 12-15

exact bonds :

4-5 5-7

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :

containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:CLASS 15:CLASS

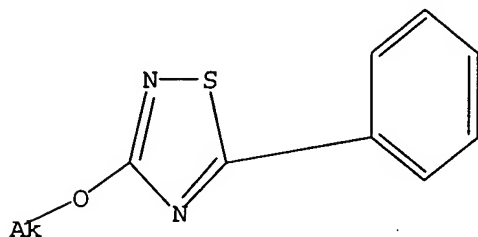


L6 STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6 STR



G1 O, S, CH2, NH, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 16

SAMPLE SEARCH INITIATED 08:35:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 34 TO ITERATE

100.0% PROCESSED 34 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 331 TO 1029

PROJECTED ANSWERS: 8 TO 329

L7 8 SEA SSS SAM L6

=> s 16 sss full

FULL SEARCH INITIATED 08:35:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 521 TO ITERATE

100.0% PROCESSED 521 ITERATIONS

102 ANSWERS

SEARCH TIME: 00.00.01

L8 102 SEA SSS FUL L6

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

166.94 339.15

FILE 'HCAPLUS' ENTERED AT 08:35:41 ON 05 NOV 2006

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FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

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=> s l8

L9 14 L8

=> d his

(FILE 'HOME' ENTERED AT 08:33:21 ON 05 NOV 2006)

FILE 'REGISTRY' ENTERED AT 08:33:34 ON 05 NOV 2006

L1 STRUCTURE UPLOADED

L2 3 S L1

L3 59 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 08:34:02 ON 05 NOV 2006

L4 13 S L3

L5 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 08:35:05 ON 05 NOV 2006

L6 STRUCTURE UPLOADED

L7 8 S L6

L8 102 S L6 SSS FULL

FILE 'HCAPLUS' ENTERED AT 08:35:41 ON 05 NOV 2006

L9 14 S L8

=> s l4 and py<=2002

22829455 PY<=2002

L10 13 L4 AND PY<=2002

=> s l9 and py<=2002

22829455 PY<=2002

L11 11 L9 AND PY<=2002

=> d l10 ibib abs hitstr tot

L10 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:900807 HCAPLUS

DOCUMENT NUMBER: 137:381259

TITLE: Preparation of 1,2,4-thiadiazole compounds and arthropodicides containing them

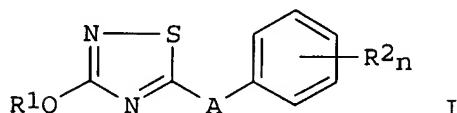
INVENTOR(S): Ihara, Hideki; Sakamoto, Noriyasu

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | KIND | DATE     | APPLICATION NO.   | DATE         |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|-------------------|--------------|
| JP 2002338557                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | A2   | 20021127 | JP 2001-152269    | 20010522 <-- |
| WO 2004041798                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | A1   | 20040521 | WO 2002-JP11644   | 20021108     |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,<br>CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,<br>GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT,<br>LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT,<br>RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG,<br>US, UZ, VN, YU, ZA, ZM, ZW<br>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,<br>KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,<br>FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,<br>CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG |      |          |                   |              |
| AU 2002368330                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | A1   | 20040607 | AU 2002-368330    | 20021108     |
| BR 2002015911                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | A    | 20050726 | BR 2002-15911     | 20021108     |
| EP 1574505                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | A1   | 20050914 | EP 2002-808100    | 20021108     |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,<br>IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |      |          |                   |              |
| CN 1688559                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | A    | 20051026 | CN 2002-829792    | 20021108     |
| US 2006167266                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | A1   | 20060727 | US 2005-530136    | 20050404     |
| PRIORITY APPLN. INFO.:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |      |          | JP 2001-152269    | A 20010522   |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |      |          | WO 2002-JP11644   | A 20021108   |
| OTHER SOURCE(S):                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |      |          | MARPAT 137:381259 |              |
| GI                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |      |          |                   |              |



AB The compds. I [R1 = C3-7 (halo)alkenyl; R2 = halo, C1-4 alkyl, C1-3 haloalkyl, C1-4 haloalkoxy, cyano, NO2; n = 0-5; A = O, S, direct bond, CR3R4, NR5; R3, R4 = H, C1-4 alkyl; R5 = H, C1-7 alkyl, C1-3 haloalkyl, C2-4 (halo)alkoxyalkyl, C3-6 (halo)alkenyl, C3-7 (halo)alkynyl, CH2CN] and arthropod control agents containing I are claimed. A composition containing 5-phenyl-3-propargyloxy-1,2,4-thiadiazole (preparation given), showed ≥90% control against *Aphis gossypii* parasitic on cucumber seedlings.

IT 476316-14-0 476316-15-1 476316-16-2  
 476316-17-3 476316-18-4 476316-19-5  
 476316-20-8 476316-21-9 476316-22-0  
 476316-23-1 476316-24-2 476316-25-3  
 476316-26-4 476316-27-5 476316-28-6  
 476316-29-7 476316-30-0 476316-31-1  
 476316-32-2 476316-33-3 476316-34-4  
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 476316-41-3 476316-43-5 476316-45-7  
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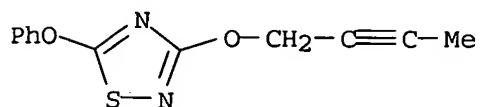
476316-59-3 476316-70-8

RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(preparation of 1,2,4-thiadiazole compds. as arthropodicides)

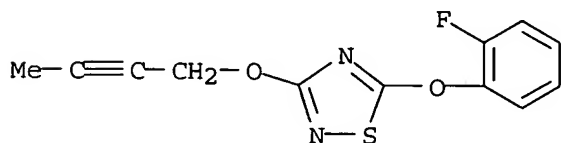
RN 476316-14-0 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-phenoxy- (9CI) (CA INDEX NAME)



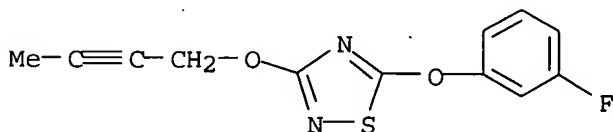
RN 476316-15-1 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-fluorophenoxy)- (9CI) (CA INDEX NAME)



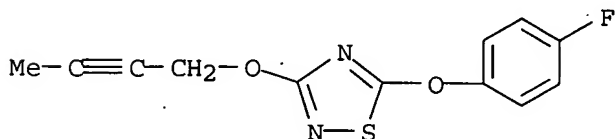
RN 476316-16-2 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-fluorophenoxy)- (9CI) (CA INDEX NAME)



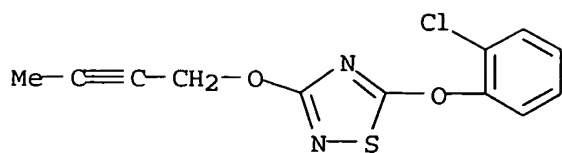
RN 476316-17-3 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)



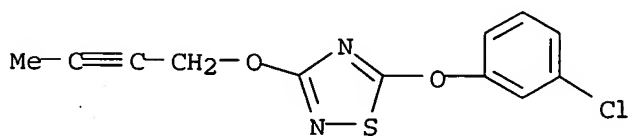
RN 476316-18-4 HCAPLUS

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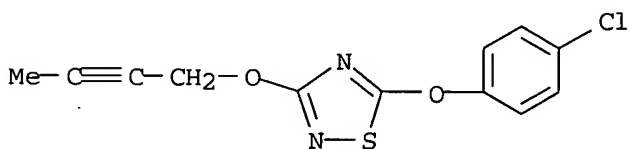
RN 476316-19-5 HCAPLUS

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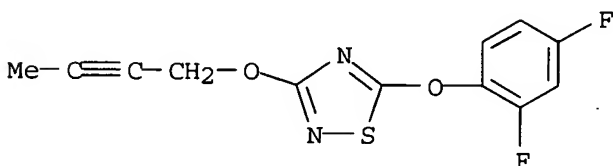
RN 476316-20-8 HCAPLUS

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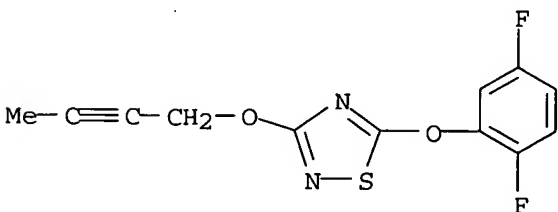
RN 476316-21-9 HCAPLUS

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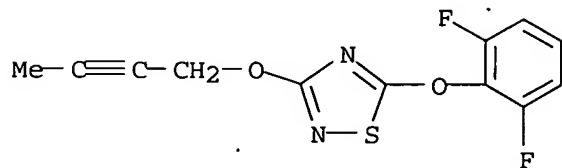


RN 476316-22-0 HCAPLUS

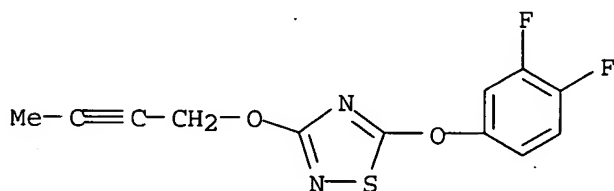
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,5-difluorophenoxy)- (9CI) (CA INDEX NAME)



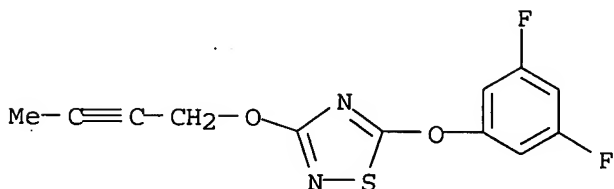
RN 476316-23-1 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,6-difluorophenoxy)- (9CI) (CA  
INDEX NAME)



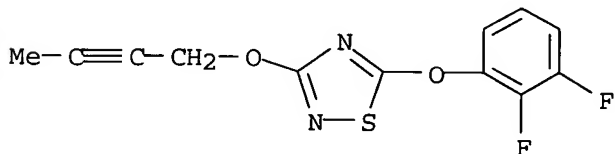
RN 476316-24-2 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,4-difluorophenoxy)- (9CI) (CA  
INDEX NAME)



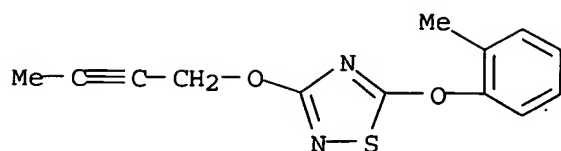
RN 476316-25-3 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,5-difluorophenoxy)- (9CI) (CA  
INDEX NAME)



RN 476316-26-4 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,3-difluorophenoxy)- (9CI) (CA  
INDEX NAME)

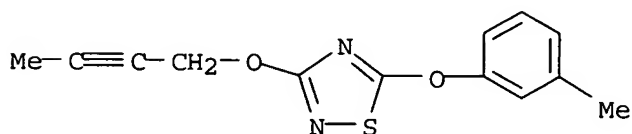


RN 476316-27-5 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-methylphenoxy)- (9CI) (CA INDEX  
NAME)



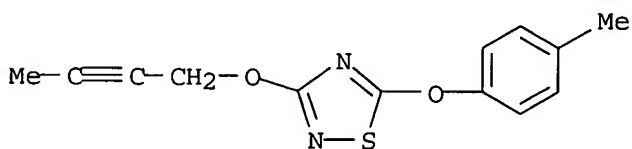
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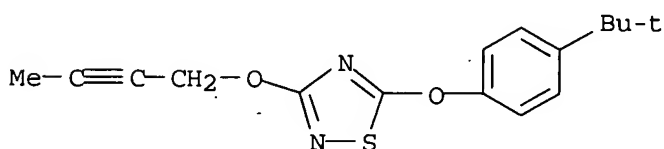
RN 476316-29-7 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-methylphenoxy)- (9CI) (CA INDEX NAME)



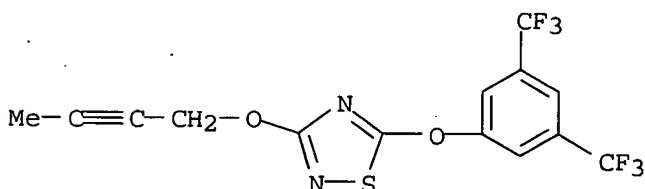
RN 476316-30-0 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[4-(1,1-dimethylethyl)phenoxy] - (9CI) (CA INDEX NAME)



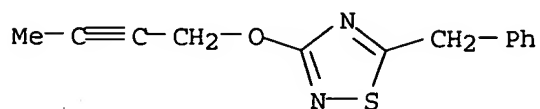
RN 476316-31-1 HCAPLUS

CN 1,2,4-Thiadiazole, 5-[3,5-bis(trifluoromethyl)phenoxy]-3-(2-butynyloxy)- (9CI) (CA INDEX NAME)



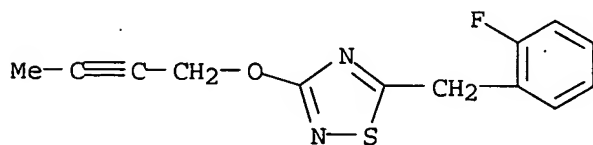
RN 476316-32-2 HCAPLUS

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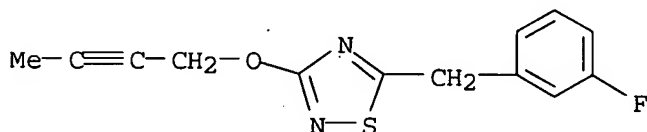
RN 476316-33-3 HCAPLUS

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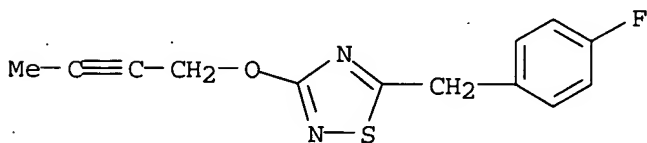
RN 476316-34-4 HCAPLUS

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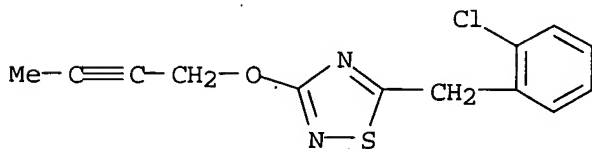
RN 476316-35-5 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)



RN 476316-36-6 HCAPLUS

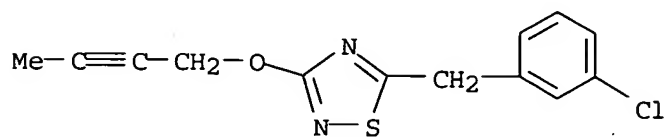
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



RN 476316-37-7 HCAPLUS

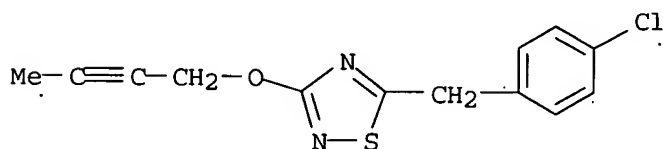


CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



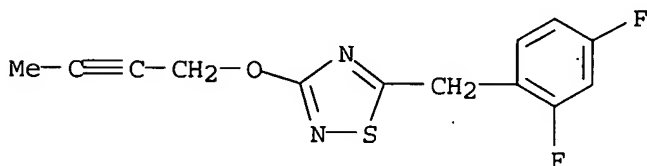
RN 476316-38-8 HCAPLUS

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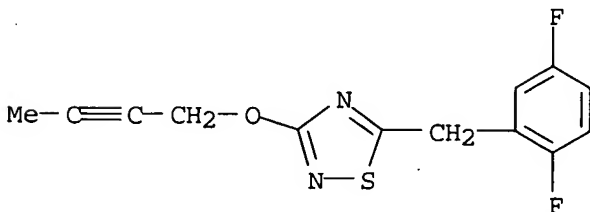
RN 476316-39-9 HCAPLUS

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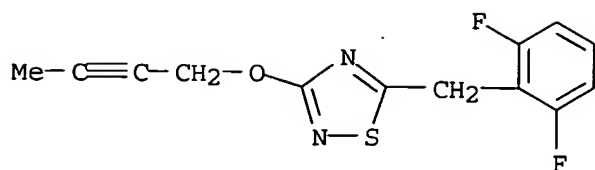
RN 476316-40-2 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2,5-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

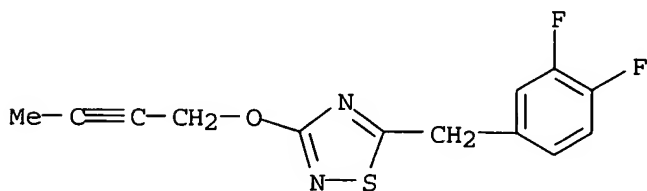


RN 476316-41-3 HCAPLUS

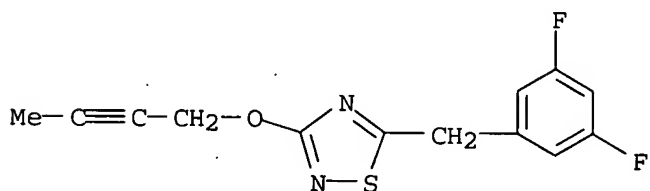
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



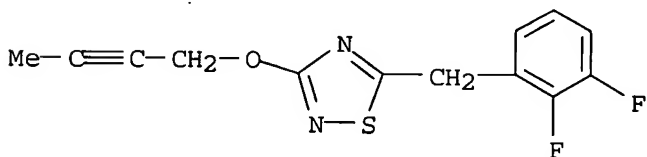
RN 476316-43-5 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3,4-difluorophenyl)methyl] - (9CI)  
(CA INDEX NAME)

RN 476316-45-7 HCAPLUS

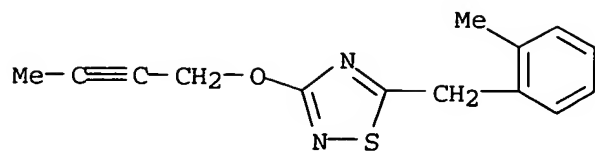
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3,5-difluorophenyl)methyl] - (9CI)  
(CA INDEX NAME)

RN 476316-47-9 HCAPLUS

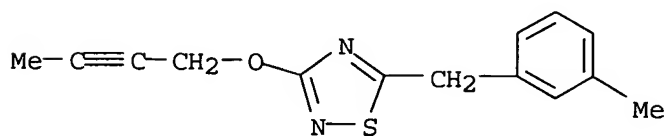
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2,3-difluorophenyl)methyl] - (9CI)  
(CA INDEX NAME)

RN 476316-49-1 HCAPLUS

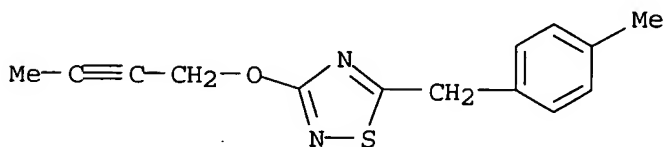
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2-methylphenyl)methyl] - (9CI) (CA  
INDEX NAME)



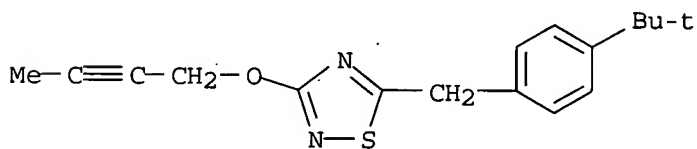
RN 476316-51-5 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



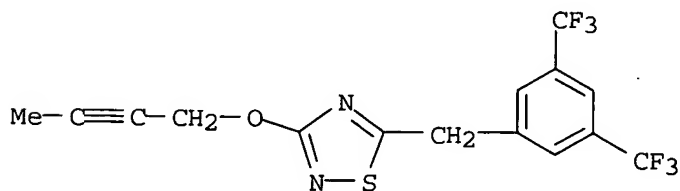
RN 476316-53-7 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 476316-55-9 HCAPLUS  
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(4-(1,1-dimethylethyl)phenyl)methyl]- (9CI) (CA INDEX NAME)

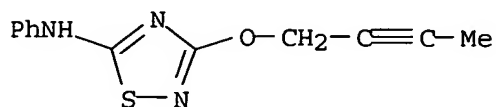


RN 476316-57-1 HCAPLUS  
CN 1,2,4-Thiadiazole, 5-[[3,5-bis(trifluoromethyl)phenyl)methyl]-3-(2-butynyloxy)- (9CI) (CA INDEX NAME)



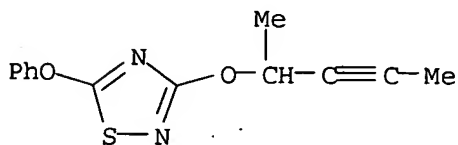
RN 476316-59-3 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, 3-(2-butynyloxy)-N-phenyl- (9CI) (CA INDEX NAME)



RN 476316-70-8 HCAPLUS

CN 1,2,4-Thiadiazole, 3-[(1-methyl-2-butynyl)oxy]-5-phenoxy- (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 13. HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:553541 HCAPLUS

DOCUMENT NUMBER: 133:163952

TITLE: Preparation of N2-phenylamidines as fungicides

INVENTOR(S): Charles, Mark David; Franke, Wilfried; Green, David Eric; Hough, Thomas Lawley; Mitchell, Dale Robert; Simpson, Donald James; Atherall, John Frederick

PATENT ASSIGNEE(S): Hoechst Schering Agrevo G.m.b.H., Germany

SOURCE: PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.                                                                 | KIND | DATE     | APPLICATION NO. | DATE         |
|----------------------------------------------------------------------------|------|----------|-----------------|--------------|
| WO 2000046184                                                              | A1   | 20000810 | WO 2000-GB345   | 20000204 <-- |
| W: AU, BR, CA, CN, CZ, HU, IL, IN, JP, KR, MX, RU, TR, UA, US, ZA          |      |          |                 |              |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE |      |          |                 |              |
| CA 2360943                                                                 | AA   | 20000810 | CA 2000-2360943 | 20000204 <-- |
| CA 2360943                                                                 | C    | 20060418 |                 |              |
| EP 1150944                                                                 | A1   | 20011107 | EP 2000-901791  | 20000204 <-- |
| EP 1150944                                                                 | B1   | 20030820 |                 |              |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI  |      |          |                 |              |
| TR 200102237                                                               | T2   | 20011221 | TR 2001-2237    | 20000204 <-- |
| BR 2000009314                                                              | A    | 20020213 | BR 2000-9314    | 20000204 <-- |
| JP 2002536354                                                              | T2   | 20021029 | JP 2000-597256  | 20000204 <-- |
| AT 247629                                                                  | E    | 20030915 | AT 2000-901791  | 20000204     |
| AU 768156                                                                  | B2   | 20031204 | AU 2000-23088   | 20000204     |
| PT 1150944                                                                 | T    | 20031231 | PT 2000-901791  | 20000204     |
| ES 2200816                                                                 | T3   | 20040316 | ES 2000-901791  | 20000204     |
| RU 2234504                                                                 | C2   | 20040820 | RU 2001-124664  | 20000204     |
| US 6893650                                                                 | B1   | 20050517 | US 2001-890775  | 20000204     |

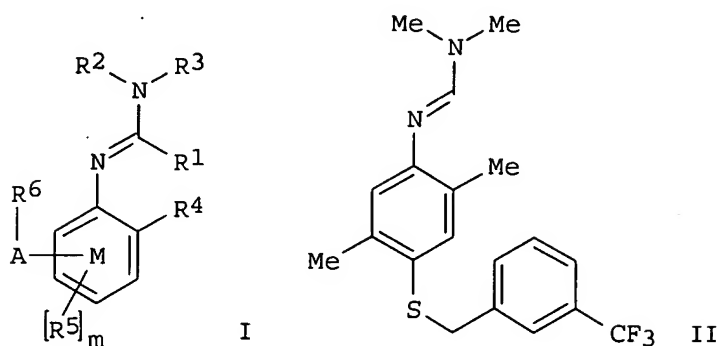
ZA 2001005845  
 HK 1043358  
 PRIORITY APPLN. INFO.:

A 20021016  
 A1 20050506  
 MARPAT 133:163952

ZA 2001-5845  
 HK 2002-105179  
 GB 1999-2592  
 WO 2000-GB345

20010716 <--  
 20020712  
 A 19990206  
 W 20000204

OTHER SOURCE(S):  
 GI



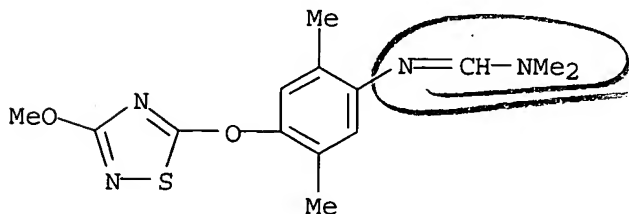
AB The title compds. [I; R1 = alkyl, alkenyl, alkynyl, etc.; R2, R3 = R1, CN, acyl, etc.; R2 and R3, or R2 and R1, together with their interconnecting atoms may form (un)substituted ring; R4 = alkyl, alkenyl, alkynyl, etc.; m = 0-3; when present R5 = R4; R6 = (un)substituted carbo- or heterocyclyl; A = a direct bond, O, C.tplbond.C, etc.; AR6 and R5 together with benzene ring M form an (un)substituted fused ring system], useful as fungicides, were prepared E.g., a 3-step preparation of the formamidine II which showed moderate to total control against Erysiphe graminis f. sp. Tritici at 500 ppm (w/v) or less, was given.

IT 287939-10-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of N2-phenylamidines as fungicides)

RN 287939-10-0 HCAPLUS

CN Methanimidamide, N'-[4-[(3-methoxy-1,2,4-thiadiazol-5-yl)oxy]-2,5-dimethylphenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

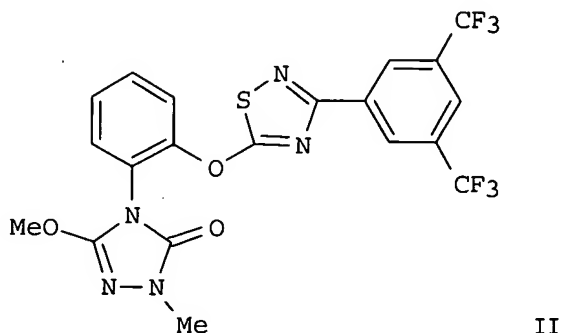
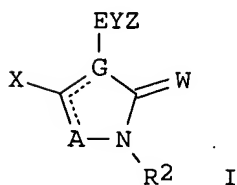
4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1998:385479 HCAPLUS

DOCUMENT NUMBER: 129:54375  
 TITLE: Arthropodicidal and fungicidal cyclic amides  
 [triazolones] and their preparation, use, and  
 compositions  
 INVENTOR(S): Brown, Richard James; Chan, Dominic Ming-Tak; Howard,  
 Michael Henry, Jr.; Daniel, Dilon Jancey; Clark, David  
 Alan; Selby, Thomas Paul  
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA  
 SOURCE: PCT Int. Appl., 232 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

| PATENT NO.                                                             | KIND | DATE             | APPLICATION NO. | DATE         |
|------------------------------------------------------------------------|------|------------------|-----------------|--------------|
| WO 9823155                                                             | A1   | 19980604         | WO 1996-US18916 | 19961126 <-- |
| W: JP, KR                                                              |      |                  |                 |              |
| RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE |      |                  |                 |              |
| ZA 9709943                                                             | A    | 19990505         | ZA 1997-9943    | 19971105 <-- |
| WO 9823156                                                             | A1   | 19980604         | WO 1997-US21944 | 19971125 <-- |
| W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU,     |      |                  |                 |              |
| ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK,        |      |                  |                 |              |
| MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA,        |      |                  |                 |              |
| US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM                     |      |                  |                 |              |
| RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,    |      |                  |                 |              |
| GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,        |      |                  |                 |              |
| GN, ML, MR, NE, SN, TD, TG                                             |      |                  |                 |              |
| AU 9854633                                                             | A1   | 19980622         | AU 1998-54633   | 19971125 <-- |
| EP 944314                                                              | A1   | 19990929         | EP 1997-948597  | 19971125 <-- |
| R: CH, DE, DK, ES, FR, GB, IT, LI, NL, IE                              |      |                  |                 |              |
| BR 9713415                                                             | A    | 20000418         | BR 1997-13415   | 19971125 <-- |
| JP 2001506984                                                          | T2   | 20010529         | JP 1998-524889  | 19971125 <-- |
| MX 9904789                                                             | A    | 20000131         | MX 1999-4789    | 19990524 <-- |
| KR 2000057254                                                          | A    | 20000915         | KR 1999-704639  | 19990526 <-- |
| PRIORITY APPLN. INFO.:                                                 |      |                  | WO 1996-US18916 | A 19961126   |
|                                                                        |      |                  | US 1996-33614P  | P 19961219   |
|                                                                        |      |                  | US 1997-48844P  | P 19970606   |
|                                                                        |      |                  | WO 1997-US21944 | W 19971125   |
| OTHER SOURCE(S):                                                       |      | MARPAT 129:54375 |                 |              |
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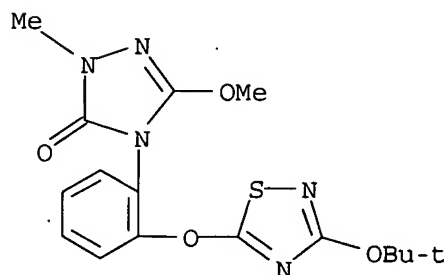


AB Title compds. I and their N-oxides and agriculturally suitable salts are disclosed [wherein E = (un)substituted 1,2-phenylene, naphthalene or heterocyclyl; A = O, S, N, NR3 or CR4; G = C or N; when G is C, then A is O, S or NR3 and the floating double bond is attached to G; and when G is N, then A is N or CR4 and the floating double bond is attached to A; W = O, S, NH, N(C1-C6 alkyl) or NO(C1-C6 alkyl); X = H, OR1, SOMR1, halo, C1-C6 alkyl, C1-C6 haloalkyl, C3-C6 cycloalkyl, cyano, NH2, NHR1, N(C1-C6 alkyl)R1, NH(C1-C6 alkoxy) or N(C1-C6 alkoxy)R1; R2 = H, C1-C6 alkyl, C1-C6 haloalkyl, C2-C6 haloalkyl, C2-C6 alkenyl, C2-C6 haloalkenyl, C2-C6 alkynyl, C2-C6 haloalkynyl, C3-C6 cycloalkyl, C2-C4 alkylcarbonyl, C2-C6 alkoxy carbonyl, hydroxy, C1-C2 alkoxy, or acetyloxy; R1 = (halo)alkyl, (halo)alkenyl, etc.; R3 = H, (halo)alkyl, etc.; Y = O, CO, SO, etc.; Z = (un)substituted alkyl, alkenyl or alkynyl, R4 = H, halo, alkyl, etc.; m = 0, 1 or 2]. Claims cover methods of arthropod and fungal control, novel compds., arthropodicidal and fungicidal compns., and novel intermediates. Approx. 1000 invention compds. were prepared For instance, 5-chloro-2,4-dihydro-4-(2-methoxyphenyl)-2-methyl-3H-1,2,4-triazol-3-one (preparation given) underwent a sequence of cleavage of the Me ether with BBr3, methoxylation of the chloride with NaOMe, and etherification of the phenolic hydroxy group with 5-chloro-3-[3,5-bis(trifluoromethyl)phenyl]-1,2,4-thiadiazole, to give title compound II. Selected I were active in screens against Erysiphe graminis, Pyricularia oryzae, Spodoptera frugiperda, Tetranychus urticae, and a variety of other standard pests.

IT 208528-37-4P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation as arthropodicide and fungicide)

RN 208528-37-4 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[2-[[3-(1,1-dimethylethoxy)-1,2,4-thiadiazol-5-yl]oxy]phenyl]-2,4-dihydro-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:112354 HCAPLUS

DOCUMENT NUMBER: 128:167436

TITLE: Preparation of arthropodicidal and fungicidal cyclic amides

INVENTOR(S): Brown, Richard James; Chan, Dominic Ming-Tak; Clark, David Alan; Drumm, Joseph Eugene, III; Koether, Gerard Michael; McCann, Stephen Frederick; Rorer, Morris Padgett; Selby, Thomas Paul; Walker, Michael Paul

PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA; Brown, Richard James; Chan, Dominic Ming-Tak; Clark, David Alan; Drumm, Joseph Eugene, III; Koether, Gerard Michael; McCann, Stephen Frederick; Rorer, Morris Padgett; Selby, Thomas Paul; Walker, Michael Paul

SOURCE: PCT Int. Appl., 130 pp.  
CODEN: PIXXD2

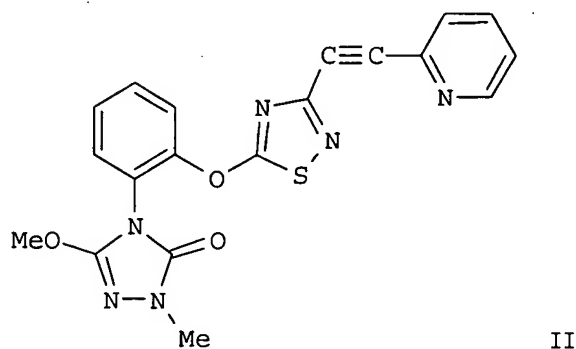
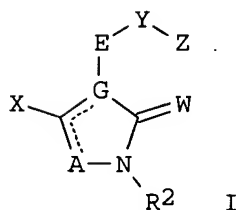
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.                                                                                                                                                                                                                                        | KIND | DATE     | APPLICATION NO.   | DATE         |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|-------------------|--------------|
| WO 9805652                                                                                                                                                                                                                                        | A2   | 19980212 | WO 1997-US12809   | 19970724 <-- |
| W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |      |          |                   |              |
| RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG                                                                                    |      |          |                   |              |
| AU 9738890                                                                                                                                                                                                                                        | A1   | 19980225 | AU 1997-38890     | 19970724 <-- |
| EP 934283                                                                                                                                                                                                                                         | A2   | 19990811 | EP 1997-936152    | 19970724 <-- |
| R: DE, FR, GB, IT                                                                                                                                                                                                                                 |      |          |                   |              |
| BR 9711816                                                                                                                                                                                                                                        | A    | 19990831 | BR 1997-11816     | 19970724 <-- |
| CN 1231663                                                                                                                                                                                                                                        | A    | 19991013 | CN 1997-198356    | 19970724 <-- |
| JP 2000516583                                                                                                                                                                                                                                     | T2   | 20001212 | JP 1998-507942    | 19970724 <-- |
| MX 9901173                                                                                                                                                                                                                                        | A    | 20000131 | MX 1999-1173      | 19990201 <-- |
| PRIORITY APPLN. INFO.:                                                                                                                                                                                                                            |      |          | US 1996-22933P    | P 19960801   |
|                                                                                                                                                                                                                                                   |      |          | WO 1997-US12809   | W 19970724   |
| OTHER SOURCE(S):                                                                                                                                                                                                                                  |      |          | MARPAT 128:167436 |              |
| GI                                                                                                                                                                                                                                                |      |          |                   |              |



AB The title compds. [I; E = (un)substituted 1,2-phenylene, naphthalene, 5-12 membered monocyclic and fused bicyclic heteroaryl; A = O, S, N, NR5, CR14; G = C, N (provided that when G = C, then A = O, S, NR5 and the floating double bond is attached to G; and when G = N, then A = N, CR14 and the floating double bond is attached to A); W = O, S, NH, N(C1-6alkyl), NO(C1-6alkyl); X = OR1, S(O)mR1, halo; Y = O, S(O)n, NR15, etc.; Z = (un)substituted C3-8 cycloalkyl, C3-8 cycloalkenyl, Ph, etc.; R1 = C1-6



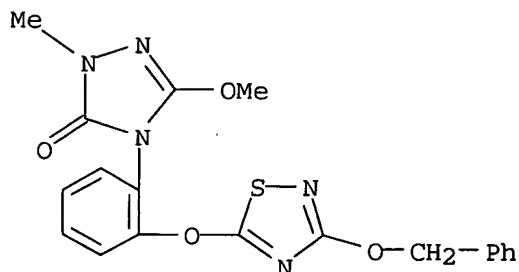
alkyl, C1-6 haloalkyl, C2-6 alkenyl, etc.; R2 = H, C1-6 alkyl, C1-6 haloalkyl, etc.; R5 = H, C1-6 alkyl, C1-6 haloalkyl, etc.; R14 = H, halo, C1-6 alkyl, etc.; R15 = H, C1-3 alkyl, C3-6 cycloalkyl, etc.; m, n = 0-2], useful for controlling plant diseases caused by fungal plant pathogens, and for controlling arthropods, were prepared Thus, reaction of 2,4-dihydro-4-(2-hydroxyphenyl)-5-methoxy-2-methyl-3H-1,2,4-triazol-3-one with 3-iodo-5-(methylsulfonyl)-1,2,4-thiadiazole in the presence of K2CO3 in Me2CO followed by reacting the resulting 2,4-dihydro-4-{2-[(3-iodo-1,2,4-thiadiazol-5-yl)oxy]phenyl}-5-methoxy-2-methyl-3H-1,2,4-triazol-3-one with 2-ethynylpyridine in the presence of CuI, PdCl2(PPh3)2 and Et3N in DMF afforded the title compound II which showed 95% control against *Erysiphe graminis* (the causal agent of wheat powdery mildew) at 500 g/ha.

IT 203054-02-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of arthropodicidal and fungicidal cyclic amides)

RN 203054-02-8 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-5-methoxy-2-methyl-4-[2-[(3-phenylmethoxy)-1,2,4-thiadiazol-5-yl]oxy]phenyl]- (9CI) (CA INDEX NAME)

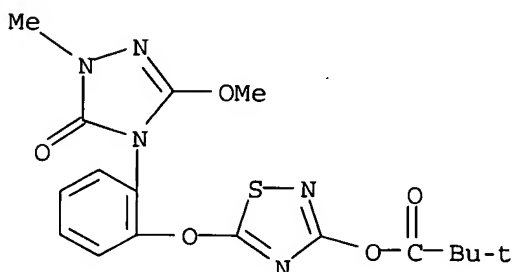


IT 203053-62-7P 203053-63-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of arthropodicidal and fungicidal cyclic amides)

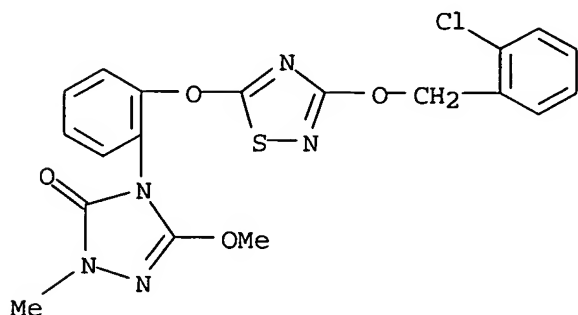
RN 203053-62-7 HCAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5-[2-(1,5-dihydro-3-methoxy-1-methyl-5-oxo-4H-1,2,4-triazol-4-yl)phenoxy]-1,2,4-thiadiazol-3-yl ester (9CI) (CA INDEX NAME)

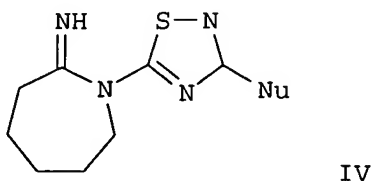
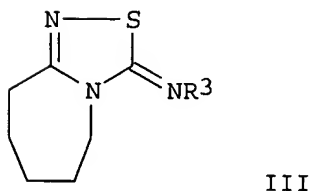
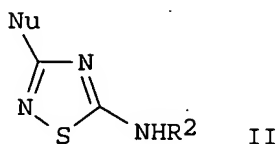
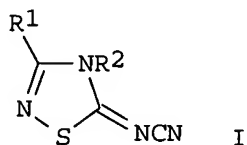


RN 203053-63-8 HCAPLUS

CN. 3H-1,2,4-Triazol-3-one, 4-[2-[[3-[(2-chlorophenyl)methoxy]-1,2,4-thiadiazol-5-yl]oxy]phenyl]-2,4-dihydro-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L10 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1995:264061 HCAPLUS  
 DOCUMENT NUMBER: 122:239609  
 TITLE: Boulton-Katritzky rearrangement of  
 5-(cyanoimino)-1,2,4-thiadiazolines  
 AUTHOR(S): Sonnenschein, Helmut; Schmitz, Ernst; Gruendemann,  
 Egon; Schroeder, Edith  
 CORPORATE SOURCE: Inst. Angewandte Chem., Berlin, D-12484, Germany  
 SOURCE: Liebigs Annalen der Chemie (1994), (12),  
 1177-80  
 CODEN: LACHDL; ISSN: 0170-2041  
 PUBLISHER: VCH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 122:239609  
 GI



AB The products of the addition of nucleophiles (alcs., amines) to the cyano group of 5-(cyanoimino)thiadiazolines I (R1 = Ph, Me, R2 = Ph, 2,6-Cl2C6H3, 3-MeC6H4, Me, Me2CHCH2) undergo a Boulton-Katritzky rearrangement. The thiadiazoles II (Nu = OMe, NMe2) are formed by subsequent nitrile elimination. In the case of bicyclic

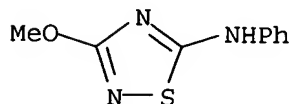
thiadiazoloazepine III (R3 = cyano), an equilibrium mixture of unrearranged iminothiadiazoline III (R3 = CR4:NH, R4 = OMe, NMe2) and rearranged thiadiazole IV is obtained as an intermediate.

IT 90564-94-6P 162231-59-6P 162231-61-0P  
162231-71-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(Boulton-Katritzky rearrangement of (cyanoimino)thiadiazolines)

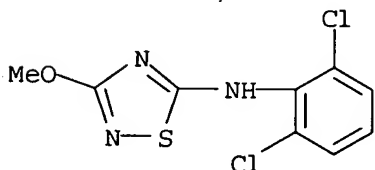
RN 90564-94-6 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



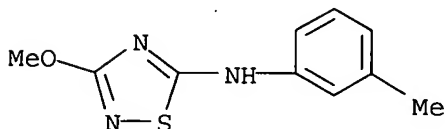
RN 162231-59-6 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, N-(2,6-dichlorophenyl)-3-methoxy- (9CI) (CA INDEX NAME)



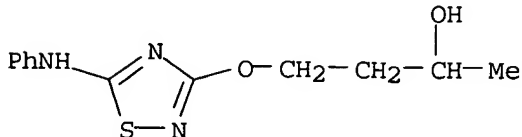
RN 162231-61-0 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-(3-methylphenyl)- (9CI) (CA INDEX NAME)



RN 162231-71-2 HCAPLUS

CN 2-Butanol, 4-[[5-(phenylamino)-1,2,4-thiadiazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



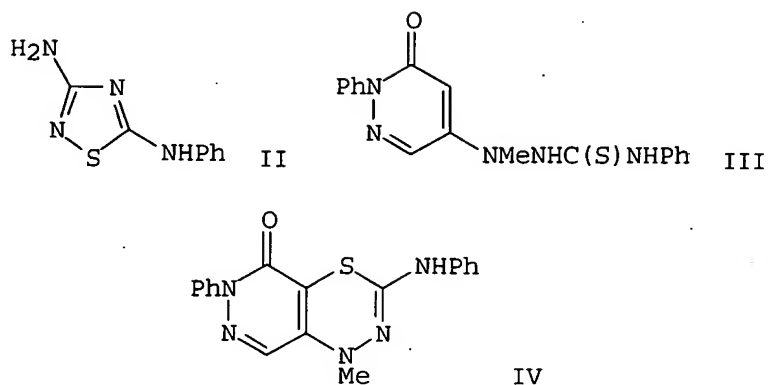
L10 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:122298 HCAPLUS

DOCUMENT NUMBER: 114:122298

TITLE: Oxidative heterocyclization using diethyl

azodicarboxylate  
 AUTHOR(S): Kihara, Yoshito; Kabashima, Shigeru; Uno, Kazue;  
 Okawara, Tadashi; Yamasaki, Tetsuo; Furukawa, Mitsuru  
 CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan  
 SOURCE: Synthesis (1990), (11), 1020-3  
 CODEN: SYNTBF; ISSN: 0039-7881  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 114:122298  
 GI



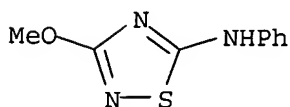
AB The reactions of amidinothioureas, imidothioureas, thioacylamidines, O-methyl-1-aryl-2-thioisobiurets, and 1-arylisodithiobiurets with di-Et azodicarboxylate (I) gave the corresponding thiadiazoles by the oxidative cyclic S-N bond formation. Thus,  $\text{H}_2\text{NC}(\text{:NH})\text{NHC}(\text{S})\text{NHPh}$  was treated with I in EtOH to give 70% thiadiazole II. Analogously, the oxidative cyclization of 2-phenyl-5-(1-methylthiosemicarbazido)-3(2H)-pyridazinones, e.g., III, with I provided 4-methyl-7-phenyl-4H-pyridazino[4,5-e][1,3,4]thiadiazin-8(7H)-ones, e.g., IV.

IT 90564-94-6P 132533-37-0P 132533-38-1P  
 132533-39-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

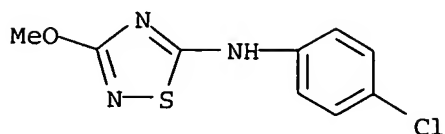
RN 90564-94-6 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)

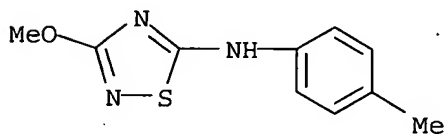


RN 132533-37-0 HCAPLUS

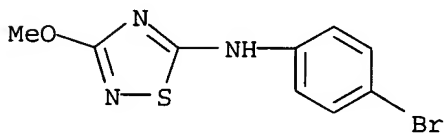
CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-methoxy- (9CI) (CA INDEX NAME)



RN 132533-38-1 HCAPLUS  
CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 132533-39-2 HCAPLUS  
CN 1,2,4-Thiadiazol-5-amine, N-(4-bromophenyl)-3-methoxy- (9CI) (CA INDEX NAME)



L10 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1986:626588 HCAPLUS  
DOCUMENT NUMBER: 105:226588  
TITLE: 1,2,4-Thiadiazole derivatives  
INVENTOR(S): Takiguchi, Daigaku; Kano, Saburo  
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 60 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.                                 | KIND | DATE     | APPLICATION NO. | DATE         |
|--------------------------------------------|------|----------|-----------------|--------------|
| WO 8602927                                 | A1   | 19860522 | WO 1985-JP617   | 19851106 <-- |
| W: AU, BR, DK, FI, JP, KR, NO, US          |      |          |                 |              |
| RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE |      |          |                 |              |
| AU 8550679                                 | A1   | 19860603 | AU 1985-50679   | 19851106 <-- |
| PRIORITY APPLN. INFO.:                     |      |          | JP 1984-234215  | A 19841108   |
|                                            |      |          | WO 1985-JP617   | A 19851106   |

GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R = Q, Q1, Q2; R1 = H, halo, alkyl, CF3C, Ph, alkoxy; n = 0-2; R2 = halo, (halo)alkyl; m = 0-2; R3 = aryl; X, X1, X2 = CH, N, N(O); Z = O, CO, NHCO, NH, alkylene, etc.; X3 = O, CH2, S, S(O)2; X4 = (CH2)4, CH:CHCH:CH; R4, R5 = H, halo, alkyl], useful as fungicides

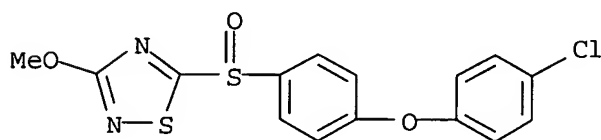
and protozoacides, were prepared Thus, a mixture of QSH (R2m = H; ZR3 = OPh-p; X = CH) and 5-Bromo-1,2,4-thiadiazole in EtOH containing NaOMe was stirred for 1/2 h in an ice bath and then heated at 50° for 2 h to give 94% I (I; R = Q; R2m = H; ZR3 = OPh-p; n = 0), whose oxidation with m-ClC6H5C(O)OOH gave 67.4% I (I; R = Q; R2m = H; ZR3 = OPh-p; n = 2). I at 0.625-1.25 µg/mL were active against Trichophyton mentagrophytes and Candida albicans.

IT 105422-76-2P 105422-77-3P 105422-90-0P  
105422-91-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as fungicide and protozoacide)

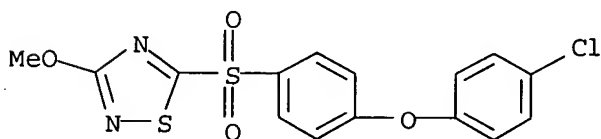
RN 105422-76-2 HCAPLUS

CN 1,2,4-Thiadiazole, 5-[[4-(4-chlorophenoxy)phenyl]sulfinyl]-3-methoxy-  
(9CI) (CA INDEX NAME)



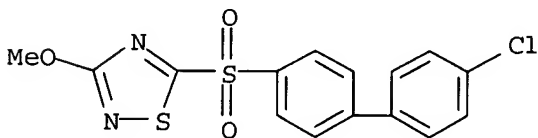
RN 105422-77-3 HCAPLUS

CN 1,2,4-Thiadiazole, 5-[[4-(4-chlorophenoxy)phenyl]sulfonyl]-3-methoxy-  
(9CI) (CA INDEX NAME)



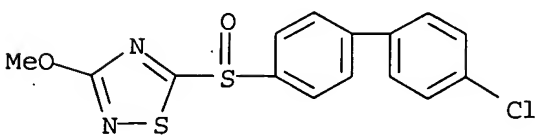
RN 105422-90-0 HCAPLUS

CN 1,2,4-Thiadiazole, 5-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-3-methoxy-  
(9CI) (CA INDEX NAME)



RN 105422-91-1 HCAPLUS

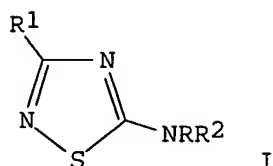
CN 1,2,4-Thiadiazole, 5-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfinyl]-3-methoxy-  
(9CI) (CA INDEX NAME)



L10 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1985:615296 HCAPLUS  
 DOCUMENT NUMBER: 103:215296  
 TITLE: 3-Substituted 5-amino-1,2,4-thiadiazoles  
 INVENTOR(S): Martin, Dieter; Graubaum, Heinz  
 PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Ger. Dem. Rep.  
 SOURCE: Ger. (East), 13 pp.  
 CODEN: GEXXA8  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND     | DATE       | APPLICATION NO. | DATE         |
|------------------------|----------|------------|-----------------|--------------|
| DD 217517              | A1       | 19850116   | DD 1983-250233  | 19830427 <-- |
| PRIORITY APPLN. INFO.: |          |            | DD 1983-250233  | 19830427     |
| OTHER SOURCE(S):       | CASREACT | 103:215296 |                 |              |

GI

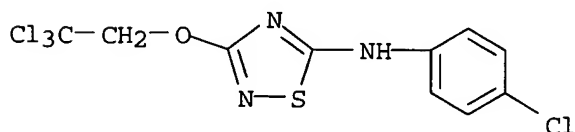


AB Thiadiazoles I [R = H, alkyl, (un)substituted aryl; R1 = CCl3, alkoxy, (un)substituted aryloxy; R2 = H, C(:NH)R1], useful as antimalarials and agricultural fungicides, herbicides, bactericides, algicides, nematocides and nitrification inhibitors (no data), were prepared by 5 methods. 5-Aminothiatriazole in an inert organic solvent was treated with PhOCN with stirring at 0-20°, then at room temperature after cessation of N evolution to give 60% I (R = R2 = H, R1 = PhO).

IT 94295-69-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as antimalarial and pesticide)

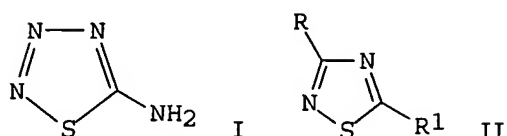
RN 94295-69-9 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-(2,2,2-trichloroethoxy)-  
 (9CI) (CA INDEX NAME)

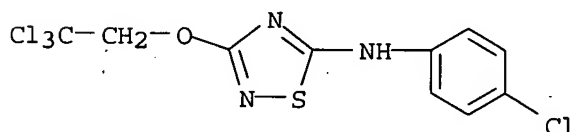


L10 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1985:504890 HCAPLUS  
 DOCUMENT NUMBER: 103:104890  
 TITLE: Synthesis of 1,2,4-thiadiazoles with potential fungistatic properties

AUTHOR(S): Martin, D.; Graubau, H.  
 CORPORATE SOURCE: Cent. Inst. Org. Chem., Ger. Acad. Sci., Berlin, DDR-1199, Ger. Dem. Rep.  
 SOURCE: Tagungsbericht - Akademie der Landwirtschaftswissenschaften der Deutschen Demokratischen Republik (1984), 222 (Syst. Fungic. Antifungal Compd.), 341-5  
 CODEN: TALDA3; ISSN: 0138-2659  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 103:104890  
 GI



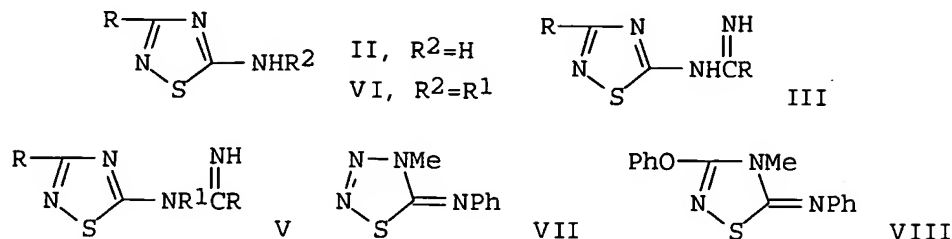
AB Treating aminothiatriazole I with RCN (R = PhO, 2-ClC<sub>6</sub>H<sub>4</sub>O, 3-, 4-MeC<sub>6</sub>H<sub>4</sub>O, 4-MeOC<sub>6</sub>H<sub>4</sub>O, Cl<sub>3</sub>C) gave 39-92% II (R<sub>1</sub> = NH<sub>2</sub>) which at 30° react further to give amidines II [R<sub>1</sub> = NHC(:NH)R]. Treating [alkyl(aryl)amino]thiatriazoles with RCN (R as above) gave II [R<sub>1</sub> = NR<sub>2</sub>C(:NH)R, R<sub>2</sub> = alkyl, aryl] which are converted to piperidino or morpholino derivs.  
 IT 94295-69-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 94295-69-9 HCAPLUS  
 CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-(2,2,2-trichloroethoxy)-(9CI) (CA INDEX NAME)



L10 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1985:166666 HCAPLUS  
 DOCUMENT NUMBER: 102:166666  
 TITLE: Cyanic acid esters. 36. 1,2,4-Thiadiazoles from amino-1,2,3,4-thiatriazoles and cyano compounds  
 AUTHOR(S): Martin, Dieter; Graubau, Heinz; Kulpe, Siegfried  
 CORPORATE SOURCE: Cent. Inst. Org. Chem., Acad. Sci., Berlin, DDR-1199, Ger. Dem. Rep.  
 SOURCE: Journal of Organic Chemistry (1985), 50(8), 1295-8  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English



OTHER SOURCE(S): CASREACT 102:166666  
GI



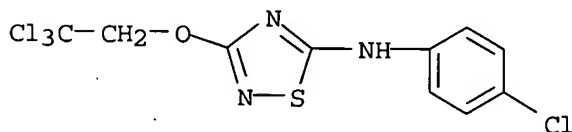
AB 5-Amino-1,2,3,4-thiadiazole (I) reacted with aryl cyanates RCN[R = R<sup>1</sup>C<sub>6</sub>H<sub>4</sub>O(R<sup>1</sup> = H, 2-Cl, 3-Me, 4-MeO)] or Cl<sub>3</sub>CCN at 0° to give 3-substituted 5-amino-1,2,4-thiadiazoles II in yields of 39-92%. Using 2 equiv of aryl cyanate at temps. approx. 40° gave 5-(iminocarbonylamino)-1,2,4-thiadiazoles III. In contrast to I, 5-alkyl(aryl)amino-1,2,3,4-thiadiazoles (IV) reacted with nitriles to give only 5-(iminocarbonylamino)-1,2,4-thiadiazoles V (R = PhO, 4-MeOC<sub>6</sub>H<sub>4</sub>O, 2,4-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>O, Cl<sub>3</sub>CCH<sub>2</sub>O, 4-MeC<sub>6</sub>H<sub>4</sub>O; R<sup>1</sup> = Me, Et, Bu, Ph, 4-ClC<sub>6</sub>H<sub>4</sub>; 4-FC<sub>6</sub>H<sub>4</sub>, 4-MeC<sub>6</sub>H<sub>4</sub>). Deacylation of V with secondary amines gave 5-alkyl(aryl)amino-1,2,4-thiadiazoles VI (R = 4-MeOC<sub>6</sub>H<sub>4</sub>O, Cl<sub>3</sub>CCH<sub>2</sub>O, PhO, Cl<sub>3</sub>C; R<sup>1</sup> = Ph, 4-ClC<sub>6</sub>H<sub>4</sub>, 4-MeC<sub>6</sub>H<sub>4</sub>, Me). The reaction of I or IV with Cl<sub>3</sub>CCN only gave the 1:1 products II or VI, resp. The 4,5-disubstituted imino-1,2,3,4-thiadiazoline VII reacted analogously to give the 4,5-disubstituted imino-1,2,4-thiadiazoline VIII.

IT 94295-69-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 94295-69-9 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-(2,2,2-trichloroethoxy)-  
(9CI) (CA INDEX NAME)



L10 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1962:473474 HCAPLUS

DOCUMENT NUMBER: 57:73474

ORIGINAL REFERENCE NO.: 57:14594a

TITLE: Thiadiazoles. XII. The ultraviolet absorption spectra of some 1,2,4-thiadiazoles

AUTHOR(S): Kurzer, Frederick; Taylor, Sheila A.

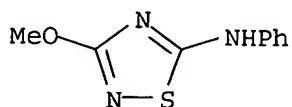
CORPORATE SOURCE: Univ. London

SOURCE: Journal of the Chemical Society (1962)  
4191-200

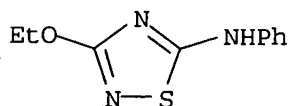
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 57:73474  
 AB cf. CA 55, 17624h. The light-absorption properties, in the near-ultraviolet region, of several 1,2,4-thiadiazoles and their acyl derivs. are described, and are discussed with a view to establishing structural correlations. Spectra are also given of amidinothiureas, thiobiurets, and dithiobiurets, which yield the 1,2,4-thiadiazoles on oxidative cyclization.  
 IT 90564-94-6, 1,2,4-Thiadiazole, 5-anilino-3-methoxy-90840-27-0, 1,2,4-Thiadiazole, 5-anilino-3-ethoxy- (spectrum of)  
 RN 90564-94-6 HCAPLUS  
 CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



RN 90840-27-0 HCAPLUS  
 CN 1,2,4-Thiadiazole, 5-anilino-3-ethoxy- (6CI, 7CI) (CA INDEX NAME)



L10 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1958:61148 HCAPLUS  
 DOCUMENT NUMBER: 52:61148  
 ORIGINAL REFERENCE NO.: 52:11016f-i,11017a-i,11018a-b  
 TITLE: Thiadiazoles. VI. 5-Amino-3-hydroxy-1,2,4-thiadiazole derivatives  
 AUTHOR(S): Kurzer, Frederick; Taylor, Sheila A.  
 CORPORATE SOURCE: Univ. London  
 SOURCE: Journal of the Chemical Society (1958) 379-86  
 CODEN: JCSOA9; ISSN: 0368-1769  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 52:61148  
 GI For diagram(s), see printed CA Issue.  
 AB cf. C.A. 51, 17895b. 1-Aryl(or alkyl)-2-thio-4-isobiurets (I), RNHCSNHC(OR'):NH, and the dealkylated 2-thiobiurets (II), RNHCSNHCNH2, were smoothly dehydrogenated by Br or H2O to 3-alkoxy(or hydroxy)-5-aryl(or alkyl)amino-1,2,4-thiadiazoles (III), RNHC:N.C(OR'):N.S. N-Aryl-N'-cyanoisothioureas (IV), RNHC(SNa):NCN, similarly afforded good yields of III (R' = H) (V). In the preparation of picrates, aqueous picric acid saturated at 30° was used. All I and II gave a precipitate of PbS when heated with Na plumbite [3N NaOH containing a few drops of 10% aqueous Pb(OAc)2] but IV resisted this reagent during 2 min. boiling. KOH (85%, 13.2 g.) in 50 ml. H2O treated successively with 22.1 g. H2NC(OMe):NH.HCl and 100 ml. Me2CO and the suspension stirred 30 min. with

20-25 g. PhNCS under reflux, the Me<sub>2</sub>CO evaporated in vacuo, the residual two-phase system stirred into 300 g. crushed ice, and the solid product crystallized once from 170 ml. 15:2 C<sub>6</sub>H<sub>6</sub>-petr. ether and from C<sub>6</sub>H<sub>6</sub> yielded 85% I (R = Ph, R' = Me) (VI), m. 129-31°. Condensation of 0.15 mole PhNCS and 0.225 mole H<sub>2</sub>NC(OEt):NH.HCl gave 23.4-26.7 g. I (R = Ph, R' = Et) (VII), m. 98-9°. VI (15.7 g.) in 150 ml. hot alc. refluxed 8-12 min. with 30 ml. concentrated HCl and the solution stirred into 1.2 l.

H<sub>2</sub>O,

the product kept 24 hrs. at 0°, and crystallized (2:1 alc.-petr. ether) gave 5.85-6.6 g. II (R = Ph) (VIII), m. 159-61°, also prepared by use of 2N alc. HCl (with persistent nauseating odor), and by hydrolysis of VII; picrate, m. 129-31° (alc.). VI (6.30 g.) in 75 ml. hot alc. cooled, the solution treated at 35-40° with 30 ml. freshly prepared ice-cold M Br in alc., the mixture poured into 750 ml. ice H<sub>2</sub>O, and the

precipitate

washed with H<sub>2</sub>O gave 75-85% III (R = Ph, R' = Me) (IX), m. 158-9° (10:3 Me<sub>2</sub>CO-EtOH), appreciably soluble in hot 3N aqueous NaOH, also obtained by treating 2.10 g. VI in 25 ml. boiling alc. with 1 ml. concentrated HCl and 5.7 ml. 6% H<sub>2</sub>O<sub>2</sub> and 2 addnl. 5.7-ml. portions H<sub>2</sub>O<sub>2</sub> at 3-min. intervals, stirring the pink turbid liquid into 150 ml. ice H<sub>2</sub>O and storing 12 hrs. at 0°, filtering, and crystallizing as above: mono-Ac derivative, m. 209-10° (Me<sub>2</sub>CO-EtOH); mono-Bz derivative, m. 180-1° (Me<sub>2</sub>CO-EtOH). Similarly, cyclizing VII with Br yielded 75-80% III (R = Ph, R' = Et) (X), m. 167-8° (alc.), also obtained in 80% yield by treating VII with H<sub>2</sub>O in the presence of mineral acid. Neither IX nor X gave a color with neutral FeCl<sub>3</sub> solution VIII (5.85 g.) in 45 ml. alc. at 35-40° treated in 1 min. with 30 ml. M Br in CHCl<sub>3</sub> (with external cooling) and the mixture added to 300 ml. H<sub>2</sub>O, the CHCl<sub>3</sub> layer evaporated at room temperature and the residual solid added to the aqueous layer, filtered,

and

the product crystallized from Me<sub>2</sub>CO-EtOH and alc. gave V (R = Ph) (XI), m. 210-12°, also produced by treating 1.95 g. VIII in 20 ml. H<sub>2</sub>O containing 0.80 g. NaOH with 8.5 ml. 6% H<sub>2</sub>O<sub>2</sub> 5 min. at 50° and filtering the cooled mixture, taking up the precipitate in 75 ml. hot H<sub>2</sub>O, and acidifying with dilute AcOH or HCl. Similarly, 1.99 g. IV (R = Ph) stirred at 45-50° in 5 ml. alc. and 3.3 ml. 3N NaOH and treated dropwise with 20 ml. 6% H<sub>2</sub>O<sub>2</sub>, the suspension kept 15 min. at 50° and diluted with 5 ml. alc., cooled to 0°, and filtered gave 42% XI. H<sub>2</sub>N<sub>2</sub>CN (4.2 g.) in 6 ml. H<sub>2</sub>O successively treated with 10 ml. 10N NaOH, 6.75 g. PhNCS, and 10 ml. alc. and the single-phase mixture heated 18 min. on a steam bath, the yellow liquid diluted with 40 ml. H<sub>2</sub>O, treated at 30-40° with 6% H<sub>2</sub>O<sub>2</sub> in 5-10 min. and kept 15 min. at 45°, the mixture cooled to 0°, and the separated Na salt acidified as above gave 5.40 g. XI; di-Bz derivative, m. 180-4°; di-Ac derivative, m. 253-5°; 3-p-tolylsulfonyloxy derivative, m. 160-2°. None of the derivs. gave a color reaction with neutral FeCl<sub>3</sub> solution XI (3.86 g.) and 6 g. Zn turnings refluxed in 60 ml. alc. and treated dropwise in 8 min. with 5 ml. concentrated HCl, the refluxing continued 4 min. and the solution decanted, the residual Zn extracted 4 times with 5 ml. alc. and the alc. extract evaporated to 1/3

volume in

vacuo, the concentrate stirred into ice H<sub>2</sub>O, and filtered gave 68% VIII, m. 157-9° (alc.). The filtrate contained no PhNH<sub>2</sub>. Similar reduction of IX gave 23% VIII and 15% PhNH<sub>2</sub>, identified as the Bz derivative. Condensation of cyanamide with 7.45 g. p-MeC<sub>6</sub>H<sub>4</sub>NCS as above and collection of the Na salt at 0°, dissoln. in 150 ml. hot H<sub>2</sub>O containing a small amount of alkali, filtration, and acidification with concentrated HCl to Congo

red

with ice cooling gave 48% V (R = p-MeC<sub>6</sub>H<sub>4</sub>), m. 212-14° (1:1 Me<sub>2</sub>CO-EtOH). Na (3.22 g.) added during 8-12 min. to 125 ml. cold anhydrous

Me<sub>2</sub>CO and the suspension stirred at 35-40° with successive addition of 14.4 g. H<sub>2</sub>NC(OMe):NH.HCl and 8.0 g. MeNCS in 10 ml. Me<sub>2</sub>CO, the stirred suspension heated to boiling 5 min. and refluxed 30-45 min., the Me<sub>2</sub>CO evaporated in vacuo and the residue diluted with 75 ml. H<sub>2</sub>O, the aqueous layer extracted

twice with 30 ml. Et<sub>2</sub>O and the exts. added to the organic layer, the mixture diluted with 100-150 ml. Et<sub>2</sub>O and washed 3 times with 10 ml. H<sub>2</sub>O, the extract dried (Na<sub>2</sub>SO<sub>4</sub>, 24 hrs.) and the filtered extract slowly treated with 28 ml. 3.5N HCl in alc., kept several hrs. at 0° and filtered, the precipitate washed with Et<sub>2</sub>O, and dried in vacuo yielded 65-72% I (R = R' = Me) (XII) HCl salt, m. 154-6°, giving a black precipitate with Na plumbite and yielding a low melting, amorphous XII; picrate, m. 154-6° (alc.). Similarly, interaction of Na, H<sub>2</sub>NC(OEt):NH.HCl, and MeNCS (with 15 min. refluxing) gave 60-70% crude HCl salt, m. 99-101°, crystallized from warm CHCl<sub>3</sub> by dilution with Et<sub>2</sub>O to give I (R = Me, R' = Et) (XIII) HCl salt, m. 105-6° (decomposition); picrate, m. 125-6° (decomposition) (alc.). Crude XIII HCl salt from 0.11 mole MeNCS treated in 30 ml. H<sub>2</sub>O with 20 ml. 3N NaOH and the solid product washed with H<sub>2</sub>O, dried, and crystallized successively from C<sub>6</sub>H<sub>6</sub> and dilute alc. yielded 62% XIII, m. 90-1°. XIII HCl salt (5.5 g.) boiled 12-15 min. in 60 ml. MeOH and 12 ml. concentrated HCl and the liquid evaporated in vacuo at 0° to 20 ml. and 5 ml. gave 3-3.5 g. product collected at both stages, purified by 3 crystns. from boiling H<sub>2</sub>O to yield 45-52% II (R = Me) (XIV), m. 174-5°. Similarly, hydrolysis of XIII in alc. in 18-20 min. yielded 68% XIV. Crude XII HCl salt (3.67 g.) in 10 ml. warm H<sub>2</sub>O treated with 20 ml. M Br in CHCl<sub>3</sub> and the aqueous layer made alkaline with 3N NaOH, cooled to 0° and filtered, the filtrate evaporated, and the residue combined with the

precipitate gave

58-68% product, crystallized successively from C<sub>6</sub>H<sub>6</sub> and MeOH to give III (R = R' = Me), m. 120-1°; picrate, m. 155-7°. Oxidation of XIII HCl salt similarly yielded 80% of the corresponding III (R = Me, R' = Et), m. 122-3° (C<sub>6</sub>H<sub>6</sub> and EtOH). XIV (1.0 g.) in 20 ml. MeOH treated with 7.5 ml. M Br in CHCl<sub>3</sub> below 30° and the mixture kept 3 hrs. at 0°, filtered and the filtrate evaporated in vacuo, the residue and the precipitate combined and taken up in 4 ml. 3N NaOH, the solution made acid to

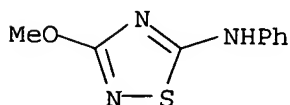
litmus

with 3N HCl, and filtered gave 0.37 g. V (R = Me), decomposing on heating and giving a purple color with FeCl<sub>3</sub>; picrate, m. 168-9° (decomposition) (1:1 H<sub>2</sub>O-EtOH); di-Bz derivative, m. 203-4° (decomposition) (Me<sub>2</sub>COEtOH).

IT 90564-94-6, 1,2,4-Thiadiazole, 5-anilino-3-methoxy-  
90840-27-0, 1,2,4-Thiadiazole, 5-anilino-3-ethoxy-  
(preparation of)

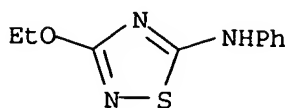
RN 90564-94-6 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)

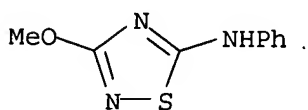


RN 90840-27-0 HCAPLUS

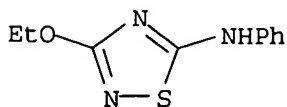
CN 1,2,4-Thiadiazole, 5-anilino-3-ethoxy- (6CI, 7CI) (CA INDEX NAME)



L10 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1957:43316 HCAPLUS  
 DOCUMENT NUMBER: 51:43316  
 ORIGINAL REFERENCE NO.: 51:8079a-b  
 TITLE: Cyclization of thiobiurets to substituted  
 1,2,4-thiadiazoles  
 AUTHOR(S): Kurzer, F.  
 CORPORATE SOURCE: Roy. Free Hosp. School Med., London  
 SOURCE: Chemistry & Industry (London, United Kingdom) (1956) 1482  
 CODEN: CHINAG; ISSN: 0009-3068  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 GI For diagram(s), see printed CA Issue.  
 AB Dealkylation of PhNHCSNHC(OR):NH (I) gave PhNHCSNHCONH2 (II), m. 159-60°; dehydrogenation of I or II with Br or H2O2 gave good yields of S.N:C(OR).N:CNHPh (III). R and m.p. were given for I: Me, 129-30°; Et, 98-9°. For III: Me, 158-9°; Et, 167-8°; H, 212-13°.  
 IT 90564-94-6, 1,2,4-Thiadiazole, 5-anilino-3-methoxy-  
 90840-27-0, 1,2,4-Thiadiazole, 5-anilino-3-ethoxy-  
 (preparation of)  
 RN 90564-94-6 HCAPLUS  
 CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



RN 90840-27-0 HCAPLUS  
 CN 1,2,4-Thiadiazole, 5-anilino-3-ethoxy- (6CI, 7CI) (CA INDEX NAME)



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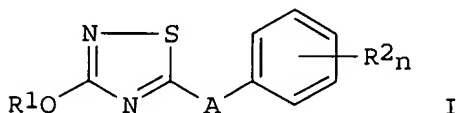
L11 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:900807 HCAPLUS  
 DOCUMENT NUMBER: 137:381259  
 TITLE: Preparation of 1,2,4-thiadiazole compounds and  
 arthropodicides containing them

11/05/2006 10530136.trn

INVENTOR(S): Ihara, Hideki; Sakamoto, Noriyasu  
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan  
SOURCE: Japan Kokai Tokkyo Koho, 13 pp.

DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.                                                                                                                                                                                                                                                                                                                                                    | KIND | DATE              | APPLICATION NO. | DATE         |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-------------------|-----------------|--------------|
| JP 2002338557                                                                                                                                                                                                                                                                                                                                                 | A2   | 20021127          | JP 2001-152269  | 20010522 <-- |
| WO 2004041798                                                                                                                                                                                                                                                                                                                                                 | A1   | 20040521          | WO 2002-JP11644 | 20021108     |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW |      |                   |                 |              |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG                                                                                                        |      |                   |                 |              |
| AU 2002368330                                                                                                                                                                                                                                                                                                                                                 | A1   | 20040607          | AU 2002-368330  | 20021108     |
| BR 2002015911                                                                                                                                                                                                                                                                                                                                                 | A    | 20050726          | BR 2002-15911   | 20021108     |
| EP 1574505                                                                                                                                                                                                                                                                                                                                                    | A1   | 20050914          | EP 2002-808100  | 20021108     |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK                                                                                                                                                                                                                                     |      |                   |                 |              |
| CN 1688559                                                                                                                                                                                                                                                                                                                                                    | A    | 20051026          | CN 2002-829792  | 20021108     |
| US 2006167266                                                                                                                                                                                                                                                                                                                                                 | A1   | 20060727          | US 2005-530136  | 20050404     |
| PRIORITY APPLN. INFO.:                                                                                                                                                                                                                                                                                                                                        |      |                   | JP 2001-152269  | A 20010522   |
|                                                                                                                                                                                                                                                                                                                                                               |      |                   | WO 2002-JP11644 | A 20021108   |
| OTHER SOURCE(S):                                                                                                                                                                                                                                                                                                                                              |      | MARPAT 137:381259 |                 |              |
| GI                                                                                                                                                                                                                                                                                                                                                            |      |                   |                 |              |



AB The compds. I [R1 = C3-7 (halo)alkenyl; R2 = halo, C1-4 alkyl, C1-3 haloalkyl, C1-4 haloalkoxy, cyano, NO2; n = 0-5; A = O, S, direct bond, CR3R4, NR5; R3, R4 = H, C1-4 alkyl; R5 = H, C1-7 alkyl, C1-3 haloalkyl, C2-4 (halo)alkoxyalkyl, C3-6 (halo)alkenyl, C3-7 (halo)alkynyl, CH2CN] and arthropod control agents containing I are claimed. A composition containing 5-phenyl-3-propargyloxy-1,2,4-thiadiazole (preparation given), showed ≥90% control against Aphis gossypii parasitic on cucumber seedlings.

IT 476315-98-7 476315-99-8 476316-00-4  
476316-01-5 476316-02-6 476316-03-7  
476316-04-8 476316-05-9 476316-06-0  
476316-07-1 476316-08-2 476316-09-3  
476316-10-6 476316-11-7 476316-12-8  
476316-13-9 476316-68-4 476316-72-0  
476316-74-2

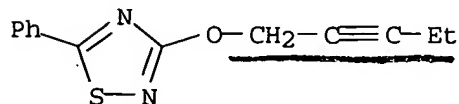
RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL

(Biological study); USES (Uses)

(preparation of 1,2,4-thiadiazole compds. as arthropodicides)

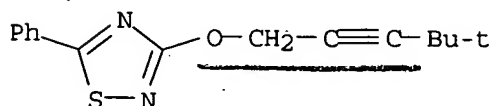
RN 476315-98-7 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-pentynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)



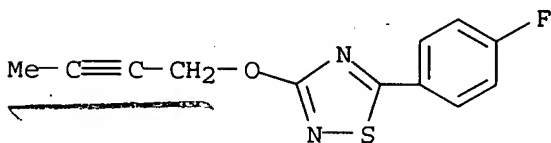
RN 476315-99-8 HCAPLUS

CN 1,2,4-Thiadiazole, 3-[(4,4-dimethyl-2-pentynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



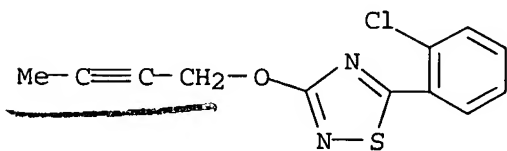
RN 476316-00-4 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



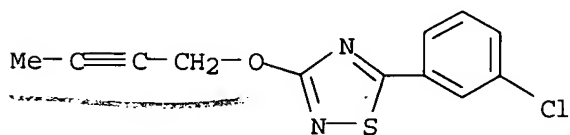
RN 476316-01-5 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 476316-02-6 HCAPLUS

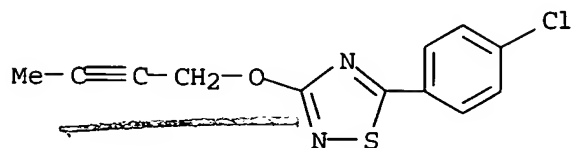
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-chlorophenyl)- (9CI) (CA INDEX NAME)



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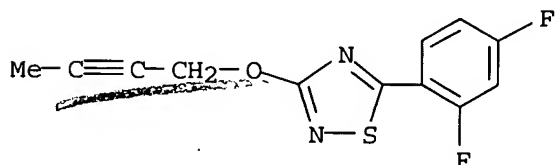
RN 476316-03-7 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



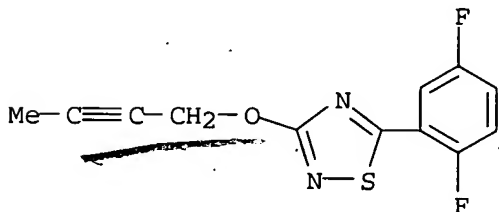
RN 476316-04-8 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)



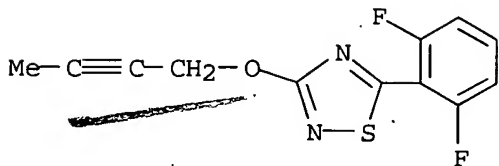
RN 476316-05-9 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,5-difluorophenyl)- (9CI) (CA INDEX NAME)



RN 476316-06-0 HCAPLUS

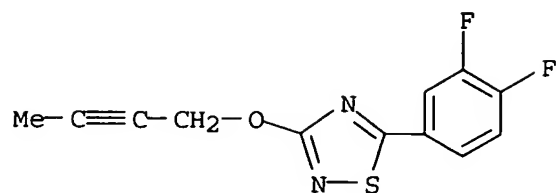
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,6-difluorophenyl)- (9CI) (CA INDEX NAME)



RN 476316-07-1 HCAPLUS

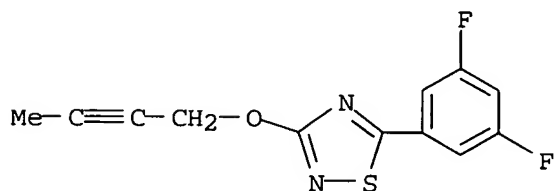
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,4-difluorophenyl)- (9CI) (CA INDEX NAME)





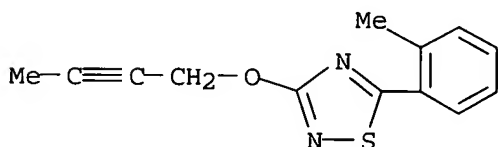
RN 476316-08-2 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,5-difluorophenyl)- (9CI) (CA INDEX NAME)



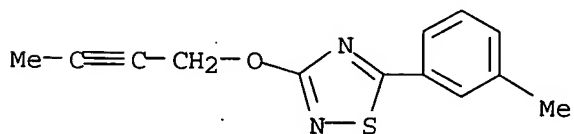
RN 476316-09-3 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)



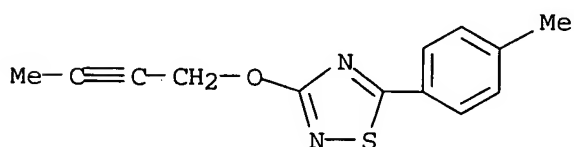
RN 476316-10-6 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-methylphenyl)- (9CI) (CA INDEX NAME)



RN 476316-11-7 HCAPLUS

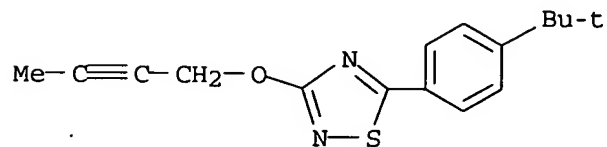
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



11/05/2006 10530136.trn

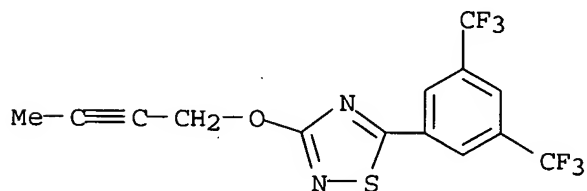
RN 476316-12-8 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[4-(1,1-dimethylethyl)phenyl]- (9CI)  
(CA INDEX NAME)



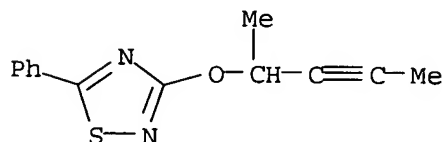
RN 476316-13-9 HCAPLUS

CN 1,2,4-Thiadiazole, 5-[3,5-bis(trifluoromethyl)phenyl]-3-(2-butynyloxy)-  
(9CI) (CA INDEX NAME)



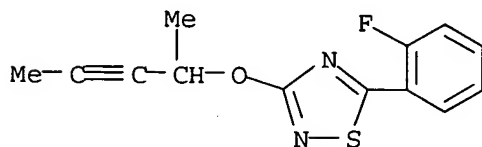
RN 476316-68-4 HCAPLUS

CN 1,2,4-Thiadiazole, 3-[(1-methyl-2-butynyl)oxy]-5-phenyl- (9CI) (CA INDEX  
NAME)



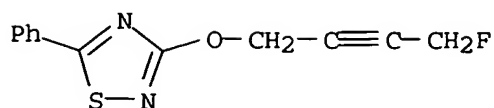
RN 476316-72-0 HCAPLUS

CN 1,2,4-Thiadiazole, 5-(2-fluorophenyl)-3-[(1-methyl-2-butynyl)oxy]- (9CI)  
(CA INDEX NAME)

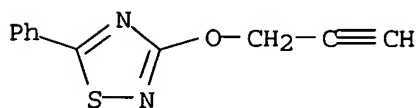


RN 476316-74-2 HCAPLUS

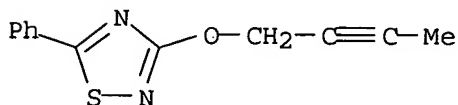
CN 1,2,4-Thiadiazole, 3-[(4-fluoro-2-butynyl)oxy]-5-phenyl- (9CI) (CA INDEX  
NAME)



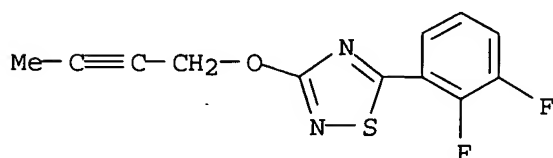
IT 476315-86-3P 476315-87-4P 476315-89-6P  
 476315-92-1P 476315-94-3P  
 RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN  
 (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (preparation of 1,2,4-thiadiazole compds. as arthropodicides)  
 RN 476315-86-3 HCAPLUS  
 CN 1,2,4-Thiadiazole, 5-phenyl-3-(2-propynyloxy)- (9CI) (CA INDEX NAME)



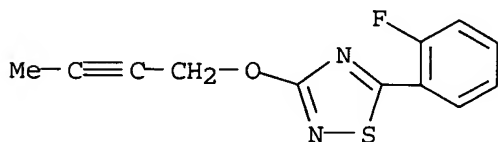
RN 476315-87-4 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)



RN 476315-89-6 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,3-difluorophenyl)- (9CI) (CA INDEX NAME)

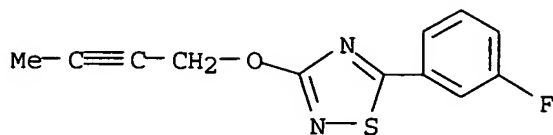


RN 476315-92-1 HCAPLUS  
 CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 476315-94-3 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-fluorophenyl)- (9CI) (CA INDEX NAME)



L11 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:738242 HCAPLUS

DOCUMENT NUMBER: 138:280905

TITLE: Anti-ischemic Compound KC 12291 Prevents Diastolic Contracture in Isolated Atria by Blockade of Voltage-Gated Sodium Channels

AUTHOR(S): Tamareille, Sophie; Le Grand, Bruno; John, Gareth W.; Feuvray, Danielle; Coulombe, Alain

CORPORATE SOURCE: Hospital Marie Lannelongue, Universite Paris Sud XI, paris, Fr.

SOURCE: Journal of Cardiovascular Pharmacology (2002), 40(3), 346-355

CODEN: JCPCDT; ISSN: 0160-2446

PUBLISHER: Lippincott Williams & Wilkins

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Several lines of evidence support a fundamental role for voltage-gated sodium channels in mediating ischemic Na rise. We examined the effect of the novel anti-ischemic compound KC 12291 on veratridine-stimulated and lysophosphatidylcholine (LPC)-induced sustained sodium current (INaL) mediated by sodium channels in isolated myocytes obtained from guinea-pig atria, by using the whole-cell patch-clamp technique. We also analyzed the effect of KC 12291 on veratridine- and LPC-induced contractures in isolated guinea-pig atria. Veratridine as well as LPC increased INaL measured at 20 ms of a 2 s pulse evoked from -100 to -30 mV (47.5 and 12 pA/pF in the presence of 40  $\mu$  veratridine and 10  $\mu$  LPC, resp., vs. 6.7 pA/pF under control conditions). A significant reduction by KC 12291 in the quantity of charge carried by veratridine-stimulated INaL in the range of test potentials between -50 mV and +10 mV was observed and similar effects were obtained on LPC-induced INaL. Thus, the quantity of charge carried by LPC-induced INaL over a 2 s pulse to -30 mV was reduced by 48% in the presence of 10  $\mu$  KC 12291 vs. a reduction by 50% of veratridine-stimulated INaL at the same test potential. Veratridine- and LPC-induced submaximal contractures in isolated atria were significantly inhibited by KC 12291 in a concentration-dependent manner, with an IC of 0.55  $\mu$  and 0.79  $\mu$ , resp. The data indicate that veratridine- and LPC-induced increases in diastolic tension are inhibited by KC 12291 by a mechanism that involves blockade of voltage-gated sodium channels mediating sustained sodium current.

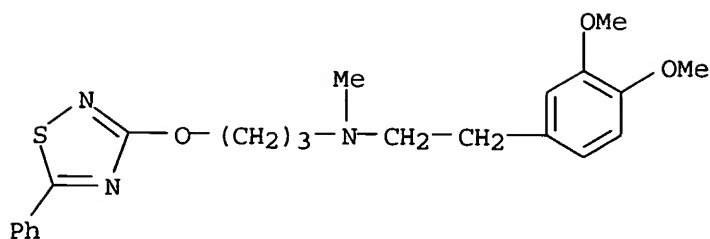
IT 181936-98-1, KC 12291

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(KC 12291 inhibits voltage-gated sodium channels and prevents diastolic contracture in atrial myocytes)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:908531 HCAPLUS

DOCUMENT NUMBER: 134:351537

TITLE: Multinuclear MR-spectroscopy on ion-homeostasis and energetics during ischemia and reperfusion

AUTHOR(S): Decking, Ulrich K. M.; Vogler, Lars; Hartmann, Matthias; Schrader, Jurgen

CORPORATE SOURCE: Department of Physiology, Heinrich-Heine-University, Dusseldorf, 40001, Germany

SOURCE: Magnetic Resonance Materials in Physics, Biology and Medicine (2000), 11(1-2), 3-4  
CODEN: MRBMEQ; ISSN: 1352-8661

PUBLISHER: Elsevier Science Ireland Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To develop a coherent model of ion homeostasis in the course of ischemia, intracellular Na<sup>+</sup>, pH and energy status as well as cardiac contractile functions were measured in the saline perfused guinea pig heart. To sensitively detect small changes of Na<sup>+</sup> upon the start of ischemia, triple quantum filtered <sup>23</sup>Na NMR spectra were acquired in the presence of shift reagent. Intracellular pH and energy status were assessed by <sup>31</sup>P NMR. The effects of Na<sup>+</sup>-H<sup>+</sup>-exchanger (NHE) inhibition were further evaluated in both stop-flow and low flow ischemia. Results showed that Na<sup>+</sup>-channels constitute a major part of Na<sup>+</sup> entry in the initial minutes following the onset of ischemia. The persistent component of the Na<sup>+</sup> current does not play a significant role in the guinea pig heart even thereafter. Due to intracellular acidification, NHE is activated and forms the dominant influx pathway in the next 30 min of ischemia, but is partially inactivated in the later course of ischemia. Alternative, not yet characterized ports of entry gain importance in this phase. Blocking either voltage-gated Na<sup>+</sup>-channels or NHE improved post-ischemic contractile function. Thus, reducing Na<sup>+</sup> overload in ischemia is a promising therapeutic approach for cardioprotection.

IT 181936-98-1, KC 12291

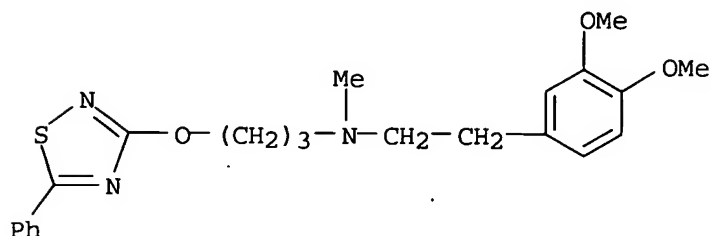
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(multinuclear MR-spectroscopy on ion-homeostasis and energetics during ischemia and reperfusion)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-

3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:97883 HCAPLUS

DOCUMENT NUMBER: 132:273796

TITLE: Primary porcine enterocyte and hepatocyte cultures to study drug oxidation reactions

AUTHOR(S) : Bader, A.; Hansen, T.; Kirchner, G.; Allmeling, C.;  
Haverich, A.; Borlak, J. T.

CORPORATE SOURCE:       Leibniz Research Laboratories for Biotechnology and  
Artificial Organs, Leibniz Research Laboratories for  
Biotechnology and Artificial Organs, Forschungszentrum  
der MHH, Hannover, D-30659, Germany

SOURCE: British Journal of Pharmacology (2000),  
129(2), 331-342

CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Primary porcine hepatocytes and enterocytes were isolated and cultured in Williams' E medium for up to 10 days to investigate potential organ differences in the metabolism of the immunosuppressive compound tacrolimus (FK 506) and of two investigational drugs (KC11346 and KC12291). Using LC-MS (FK506) and HPLC-FL (KC 11346/12291) a number of metabolites with identical mass and/or identical retention time could be detected. In the case of tacrolimus hepatocytes and enterocytes produced the same spectrum of metabolites, e.g. bisdemethyl-tacrolimus, demethyl-tacrolimus, demethyl-hydroxy-tacrolimus and hydroxy-tacrolimus, albeit at varying intensities. Treatment of enterocyte cultures with dexamethasone increased the overall metabolite formation very significantly (up to 36 fold). The metabolism of tacrolimus was also studied with preps. of insect cells, that express specifically high levels of individual human cytochrome P 450 (CYP) isoenzymes. All metabolites could be generated with microsomal preps. specifically expressing CYP3A4, but hydroxytacrolimus was exclusively produced by CYP3A5. In the case of the investigational drugs KC 11346 and KC 12291 only three metabolites were formed by cultured enterocytes whereas hepatocytes produced 10 and 20 metabolites, resp. When assessed at the protein level CYP1A and CYP3A were expressed in cultures of porcine enterocytes for up to 10 days but porcine hepatocytes expressed addnl. CYP2C9/10. In conclusion, primary enterocytes and hepatocytes can be successfully cultured for several days

while maintaining mono-oxygenase activity and may therefore be used as a tool for studying intestinal and hepatic metabolism

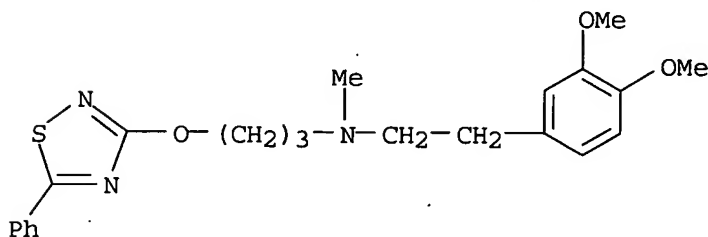
IT 181936-98-1, KC12291

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(biotransformation of tacrolimus and other drugs in primary porcine enterocyte vs. hepatocyte cultures)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:691080 HCAPLUS

DOCUMENT NUMBER: 130:148417

TITLE: Cardioprotective actions of KC 12291. II. Delaying Na<sup>+</sup> overload in ischemia improves cardiac function and energy status in reperfusion

AUTHOR(S): Hartmann, Matthias; Decking, U. K. M.; Schrader, Jurgen

CORPORATE SOURCE: Institut fur Herz- und Kreislaufphysiologie, Heinrich-Heine-Universitat Dusseldorf, Postfach 10 10 07, Dusseldorf, D-40001, Germany

SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1998), 358(5), 554-560

CODEN: NSAPCC; ISSN: 0028-1298

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The novel blocker of voltage-gated Na<sup>+</sup> channels KC 12291 (1-(5-phenyl-1,2,4-thiadiazol-3-yl-oxypropyl)-3-[N-methyl-N-[2-(3,4-dimethoxyphenyl)ethyl] amino] propane hydrochloride) delays myocardial Na<sup>+</sup> overload in ischemia. To test whether KC 12291 displays cardioprotective properties in the intact heart, cardiac function, energy status and intracellular pH (31P NMR) as well as ion homeostasis (23Na NMR) were investigated during low-flow ischemia (100 µl/min for 36 min) followed by reperfusion. In the well-oxygenated, isolated perfused guinea pig heart, KC 12291 (1 µM) had no effect on left ventricular developed pressure (LVDP; 54±19 mmHg). KC 12291 delayed the onset and decreased the extent of ischemic contracture and markedly improved the recovery of LVDP in reperfusion [39±14 mmHg (n=4) vs 2±2 mmHg in controls (n=5)]. KC 12291 did not influence the rapid drop in phosphocreatine

(PCr) following onset of ischemia but attenuated the decline in ATP. It also diminished the ischemia-induced fall in intracellular pH [ $6.39 \pm 0.2$  ( $n=6$ ) vs  $6.18 \pm 0.20$  in controls ( $n=6$ )]. In reperfusion, KC 12291 remarkably enhanced the recovery of PCr ( $84.8 \pm 9.6\%$  vs  $51.1 \pm 8.8\%$  of baseline) and ATP ( $38.2 \pm 12.9\%$  vs  $23.7 \pm 9.3\%$  of baseline). It also accelerated the recovery of intracellular pH. KC 12291 not only reduced the extent of ischemia-induced  $\text{Na}^+$  overload, but also enhanced  $\text{Na}^+$  recovery. It is concluded that KC 12291 delays contracture and reduces ATP depletion and acidosis in ischemia, and markedly improves the functional, energetic and ionic recovery in reperfusion. Blocking voltage-gated  $\text{Na}^+$  channels in ischemia to delay  $\text{Na}^+$  overload may thus constitute a promising therapeutic approach for cardioprotection.

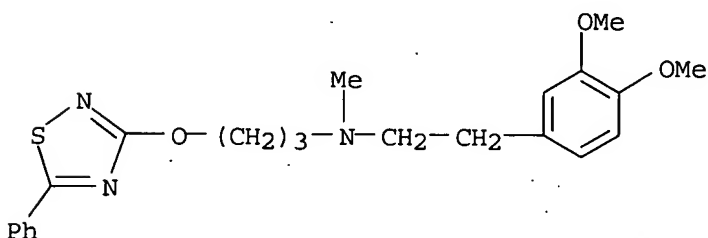
IT 181936-98-1, KC 12291

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(cardioprotective actions of KC 12291: delaying  $\text{Na}^+$  overload in ischemia improves cardiac function and energy status in reperfusion)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:691078 HCAPLUS

DOCUMENT NUMBER: 130:162913

TITLE: Cardioprotective actions of KC 12291 I. Inhibition of voltage-gated  $\text{Na}^+$  channels in ischemia delays myocardial  $\text{Na}^+$  overload

AUTHOR(S): Decking, U. K. M.; Hartmann, Matthias; Rose, Horst; Bruckner, Reinhard; Meil, Jorg; Schrader, Jurgen

CORPORATE SOURCE: Institut fur Herz- und Kreislaufphysiologie, Heinrich-Heine-Universitat Dusseldorf, Postfach 10 10 07, Dusseldorf, D-40001, Germany

SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1998), 358(5), 547-553

CODEN: NSAPCC; ISSN: 0028-1298

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To characterize KC 12291 (1-(5-phenyl-1,2,4-thiadiazol-3-yl-oxypropyl)-3-[N-methyl-2-(3,4-dimethoxyphenyl) ethyl] amino] propane hydrochloride), a



newly synthesized inhibitor of voltage-gated Na<sup>+</sup> channels, the effects of the agent on Na<sup>+</sup> current and ischemia-induced Na<sup>+</sup> overload were investigated in isolated cardiomyocytes, atria and saline-perfused hearts. As measured by the patch clamp technique, KC 12291 (1 μM) significantly reduced peak Na<sup>+</sup> current after activation of voltage-gated Na<sup>+</sup> channels in rat cardiomyocytes. Partial depolarization enhanced the inhibitory effects during steady state conditions of the channel. In isolated guinea pig atria, 1 μM KC 12291 had no effect on contractility under basal conditions but effectively delayed the onset and reduced the extent of anoxic contracture. The concentration-response curve was clearly shifted to

the

left when atria were partially depolarized by increased extracellular K<sup>+</sup>. As measured by <sup>23</sup>Na NMR spectroscopy in isolated perfused guinea pig hearts, intracellular Na<sup>+</sup> rose more than four-fold in a linear fashion during 60 min of low-flow ischemia. KC 12291 (1 μM) prevented Na<sup>+</sup> overload within the initial 12 min of ischemia; thereafter the slope of Na<sup>+</sup> accumulation was identical to controls. Elec. excitability of hearts, evaluated by intracardial ECG, completely ceased within 15 min after the onset of ischemia. KC 12291 (1 μM) accelerated this process by more than 6 min. The data provide first evidence that KC 12291 reduces Na<sup>+</sup> influx through voltage-gated Na<sup>+</sup> channels during ischemia and thus delays Na<sup>+</sup> overload by enhancing the inexcitability of the heart.

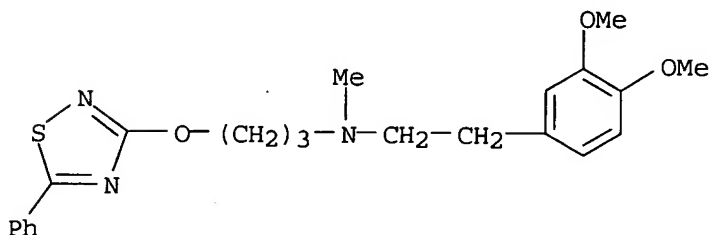
IT 181936-98-1, KC 12291

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(cardioprotective actions of KC 12291: inhibition of voltage-gated sodium channels in ischemia delays myocardial sodium overload)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:55258 HCAPLUS

DOCUMENT NUMBER: 128:212570

TITLE: Sensitive method for the determination of KC 12291 in rat plasma and urine by high-performance liquid chromatography

AUTHOR(S): Tomori, E.; Tormasi, E.; Varga, M.; Borlak, J.

CORPORATE SOURCE: Institute for Drug Research Ltd., P.O. Box 82, Budapest, H-1325, Hung.

SOURCE: Journal of Chromatography, B: Biomedical Sciences and Applications (1998), 705(1), 105-110  
 CODEN: JCBEP; ISSN: 0378-4347  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

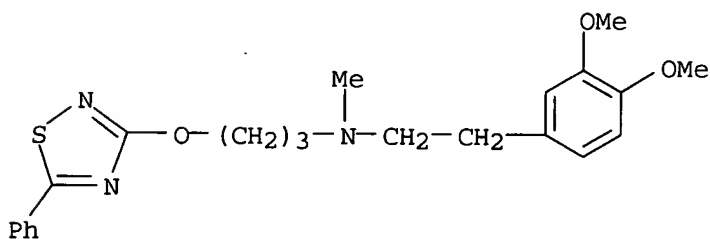
AB A sensitive and selective ion-pair reversed-phase HPLC method has been developed for the quant. determination of KC 12291 and its major metabolite, KC 13194, in rat plasma and urine. An Ultrasphere ODS column constructed by using a mobile phase of 1 mM 1-octanesulfonic acid containing acetonitrile-0.1 M triethylamine phosphate buffer, pH 2.2 (29:71, volume/volume in plasma and 27:73, volume/volume in urine), an internal standard and a fluorescent detector (excitation 265 nm, emission 370 nm) were used for the separation and the quant. determination, resp. The plasma samples were made alkaline and both compds.

were cleaned up by the use of liquid-liquid extraction The limit of quantification was 10 ng/mL for KC 12291 in plasma and urine and for KC 13194 and 100 ng/mL in plasma, resp. The assay has been validated with respect to system suitability, accuracy, precision, recovery, stability and ruggedness. All validated parameters were found to be within the necessary limits.

IT 181936-98-1, KC 12291 181938-50-1, KC 13194  
 RL: ANT (Analyte); ANST (Analytical study)  
 (KC 12291 and its metabolite KC 13194 determination in plasma and urine by HPLC)

RN 181936-98-1 HCAPLUS

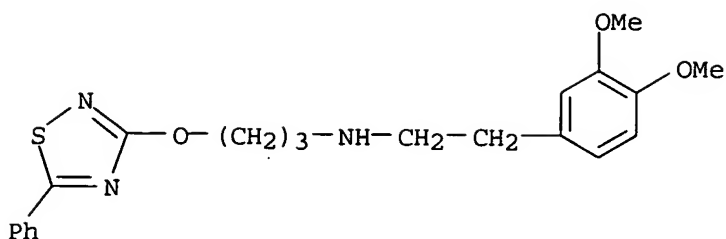
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-50-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:537795 HCAPLUS

DOCUMENT NUMBER: 125:247807

TITLE: (Phenylalkylaminoalkyloxy)-heteroaryl compounds having heart-rate-lowering and anti-ischemic effects

INVENTOR(S): Kehrbach, Wolfgang; Mlinaric, Michael; Ziegler, Dieter; Brueckner, Reinhard; Bielenberg, Willi

PATENT ASSIGNEE(S): Kali-Chemie Pharma GmbH, Germany

SOURCE: U.S., 34 pp., Cont.-in-part of U.S. Ser. No. 352, 353, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO.                                                            | KIND | DATE     | APPLICATION NO.  | DATE         |
|-----------------------------------------------------------------------|------|----------|------------------|--------------|
| US 5547967                                                            | A    | 19960820 | US 1995-476118   | 19950607 <-- |
| DE 4341749                                                            | A1   | 19950614 | DE 1993-4341749  | 19931208 <-- |
| DE 19513503                                                           | A1   | 19961017 | DE 1995-19513503 | 19950410 <-- |
| US 5679699                                                            | A    | 19971021 | US 1995-576699   | 19951221 <-- |
| EP 737680                                                             | A1   | 19961016 | EP 1996-105335   | 19960403 <-- |
| EP 737680                                                             | B1   | 20040303 |                  |              |
| R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE |      |          |                  |              |
| AT 260905                                                             | E    | 20040315 | AT 1996-105335   | 19960403     |
| ES 2213165                                                            | T3   | 20040816 | ES 1996-105335   | 19960403     |
| JP 09151180                                                           | A2   | 19970610 | JP 1996-88590    | 19960410 <-- |
| PRIORITY APPLN. INFO.:                                                |      |          |                  |              |
|                                                                       |      |          | DE 1993-4341749  | A 19931208   |
|                                                                       |      |          | US 1994-352353   | B2 19941208  |
|                                                                       |      |          | DE 1995-19513503 | A 19950410   |
|                                                                       |      |          | US 1995-476118   | A3 19950607  |

OTHER SOURCE(S): MARPAT 125:247807  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 3-(Phenylalkylaminoalkyloxy)heteroaryl compds. having heart rate lowering

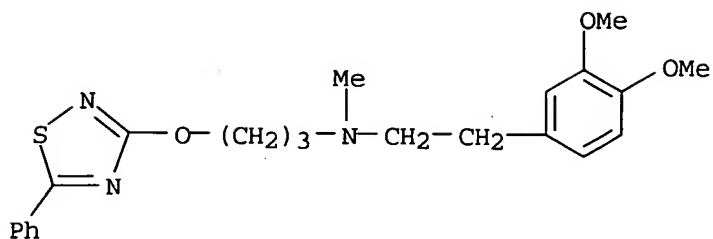
and/or anti-ischemic effects, methods for their preparation and pharmaceutical compns. containing them are described. The compds. correspond to the general formula I in which n is an integer from 1-5, A = NR<sub>1</sub>Q in which R<sub>1</sub> represents hydrogen or a lower alkyl group and Q represents a (CH<sub>2</sub>)<sub>m</sub> group in which m is 2 to 8 and which may optionally be substituted in the α position to the oxygen atom by 1 or 2 lower alkyl groups, or Q represents a 2-hydroxypropylene chain, or A = [cyclic N(CH<sub>2</sub>)<sub>p</sub>]-B in which p is 4 to 6 and B represents a (CH<sub>2</sub>)<sub>r</sub> group in which r is 1 to 3 and which may optionally be substituted in the α position to the oxygen atom by 1 or 2 lower alkyl groups; R<sub>2</sub> = e.g., H, halogen, lower alkyl; R<sub>3</sub> = e.g., H, halogen, lower alkyl; R<sub>4</sub> = H or lower alkyl; R<sub>5</sub> is disposed in the 1 or 2 position and represents hydrogen, lower alkyl or a phenyl-lower alkyl group; R<sub>6</sub> = e.g., H, lower alkyl, lower alkoxy; R<sub>7</sub> = e.g., H, lower alkyl, lower alkoxy, and their acid addition salts. The compds. also correspond to the general formula II wherein R<sub>1</sub> = H or lower alkyl; R<sub>2</sub> = e.g., H, halo, lower alkyl; R<sub>3</sub> = e.g., H, halo, lower alkyl; R<sub>4</sub> = thienyl or R<sub>5</sub>R<sub>6</sub>-substituted Ph wherein R<sub>5</sub> = e.g., H, halo, lower alkyl and R<sub>6</sub> = e.g., H, halo, lower alkyl; A = N or R<sub>7</sub>C in which R<sub>7</sub> = H or lower alkyl; B = O or, if A = N, also S; n = an integer from 1-5; and Q = (CH<sub>2</sub>)<sub>m</sub> where m is an integer from 2-8 and which may optionally be substituted by a lower alkyl, or represents the 2-hydroxypropylene chain, or a physiol. acceptable acid addition salt thereof. Thus, e.g., alkylation of 5-(3,4-dimethoxyphenyl)pyrazolin-3-one (preparation given) with 3-[N-(2-(3,4-dimethoxyphenyl)ethyl)-N-methylamino]propyl chloride (preparation given) afforded aminoalkoxypyrazole III which exhibited FRQ 75 (that concentration, in μmol/L, at which 20 min after the administration of the substance there is a reduction in the heart rate to 75% of the initial value) = 1.6. Data were also presented for cytoprotective effect on atrial contraction induced by hypoxia (as low as 0.55 μM), and for corresponding force recovery after hypoxia (up to 80%). Pharmaceutical formulations were given.

IT 181935-23-9P 181935-25-1P 181935-26-2P  
 181935-28-4P 181935-29-5P 181935-31-9P  
 181935-32-0P 181935-37-5P 181936-98-1P  
 181937-06-4P 181937-10-0P 181937-18-8P  
 181937-24-6P 181937-26-8P 181937-28-0P  
 181937-36-0P 181937-41-7P 181937-74-6P  
 181938-14-7P 181938-16-9P 181938-19-2P  
 181938-22-7P 181938-25-0P 181938-28-3P  
 181938-34-1P 181938-39-6P 181938-41-0P  
 181938-43-2P 181938-45-4P 181938-50-1P  
 181938-57-8P 181938-59-0P 181938-60-3P  
 181938-61-4P 181938-64-7P 181938-66-9P  
 181938-71-6P 181938-73-8P 181938-75-0P  
 181954-84-7P 181954-88-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 ((phenylalkylaminoalkyloxy)-heteroaryl compds. having heart-rate-lowering and anti-ischemic effects)

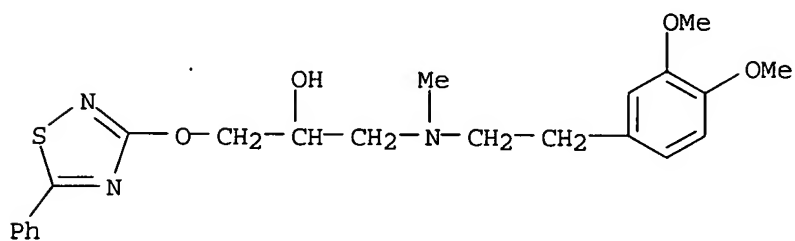
RN 181935-23-9 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]- (9CI) (CA INDEX NAME)



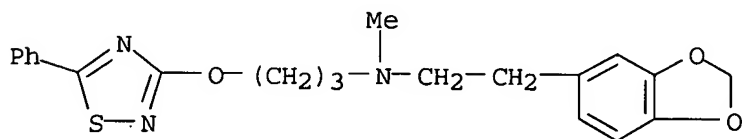
RN 181935-25-1 HCAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]- (9CI) (CA INDEX NAME)



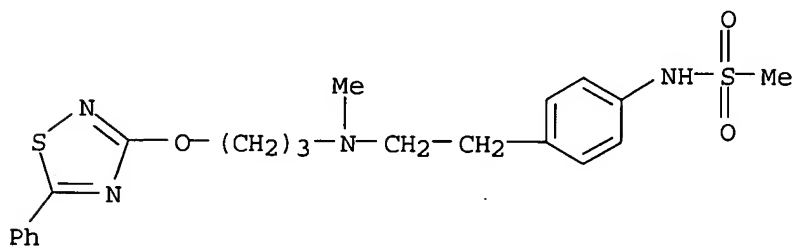
RN 181935-26-2 HCAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]- (9CI) (CA INDEX NAME)



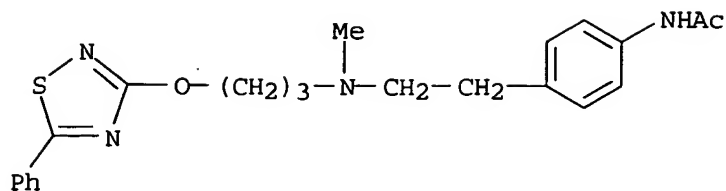
RN 181935-28-4 HCAPLUS

CN Methanesulfonamide, N-[4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]- (9CI) (CA INDEX NAME)



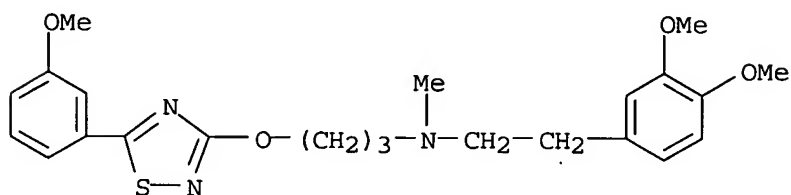
RN 181935-29-5 HCAPLUS

CN Acetamide, N-[4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]- (9CI) (CA INDEX NAME)



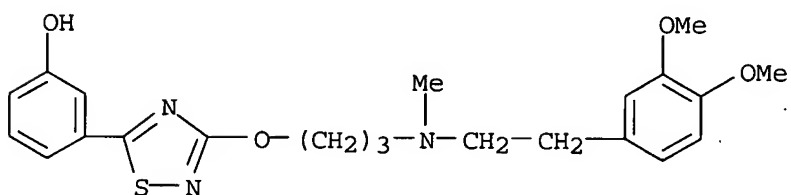
RN 181935-31-9 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[(5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl)oxy]propyl]-N-methyl- (9CI) (CA INDEX NAME)



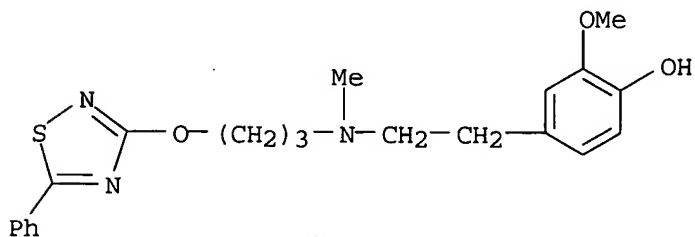
RN 181935-32-0 HCAPLUS

CN Phenol, 3-[3-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propoxy]-1,2,4-thiadiazol-5-yl]- (9CI) (CA INDEX NAME)



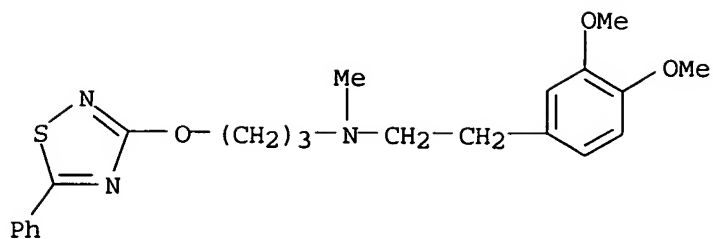
RN 181935-37-5 HCAPLUS

CN Phenol, 2-methoxy-4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 181936-98-1 HCAPLUS

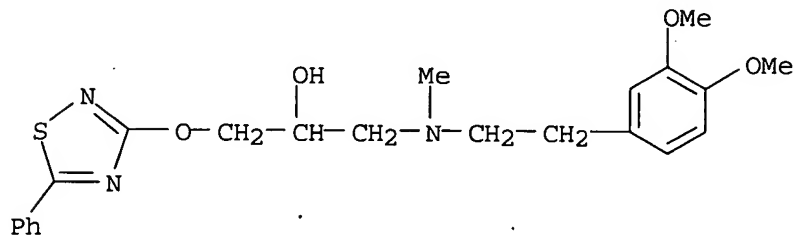
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181937-06-4 HCAPLUS

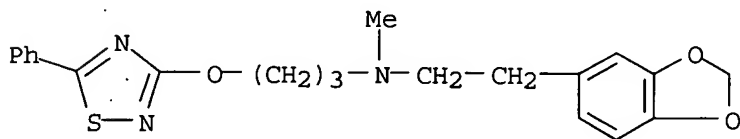
CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181937-10-0 HCAPLUS

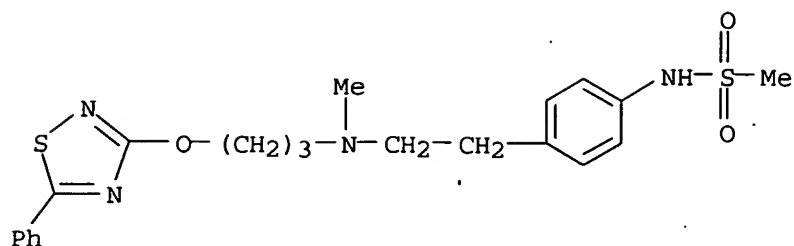
CN 1,3-Benzodioxole-5-ethanamine, N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181937-18-8 HCAPLUS

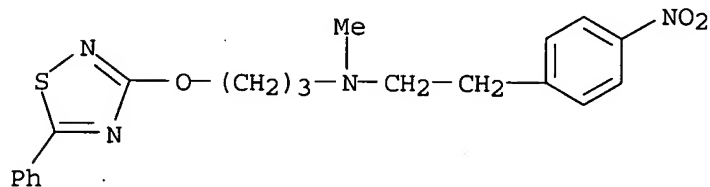
CN Methanesulfonamide, N-[4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181937-24-6 HCAPLUS

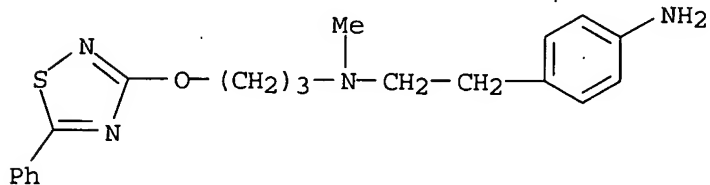
CN Benzeneethanamine, N-methyl-4-nitro-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181937-26-8 HCAPLUS

CN Benzeneethanamine, 4-amino-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

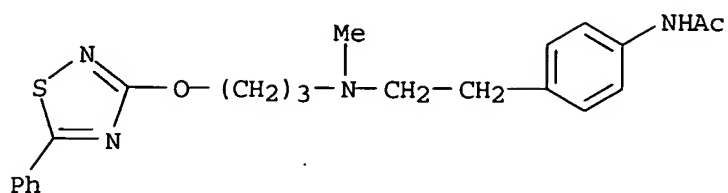


● HCl

RN 181937-28-0 HCAPLUS

CN Acetamide, N-[4-[2-[methyl 3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

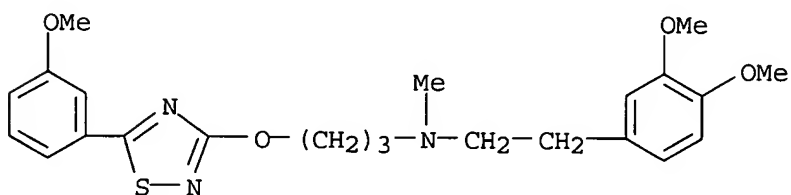




● HCl

RN 181937-36-0 HCAPLUS

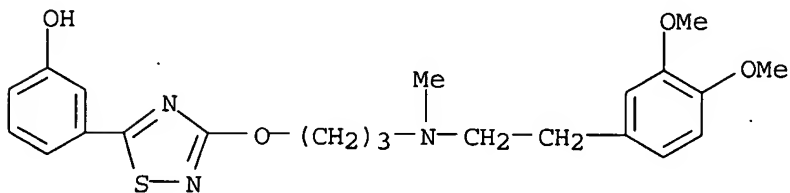
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[[5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181937-41-7 HCAPLUS

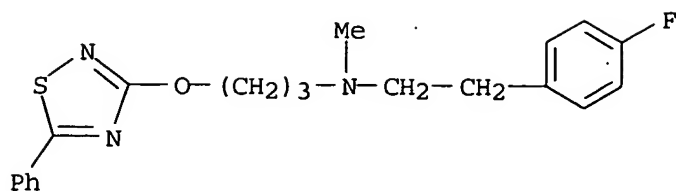
CN Phenol, 3-[3-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propoxy]-1,2,4-thiadiazol-5-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181937-74-6 HCAPLUS

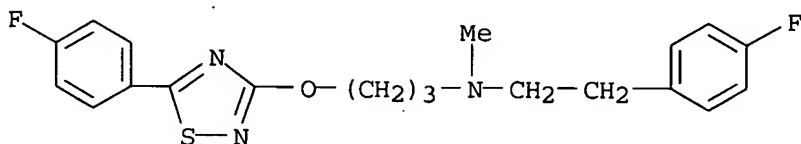
CN Benzeneethanamine, 4-fluoro-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-14-7 HCAPLUS

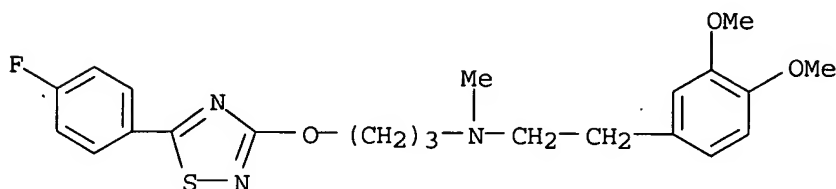
CN Benzenethanamine, 4-fluoro-N-[3-[[5-(4-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-16-9 HCAPLUS

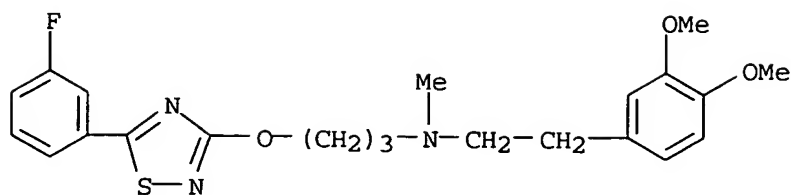
CN Benzenethanamine, N-[3-[[5-(4-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-19-2 HCAPLUS

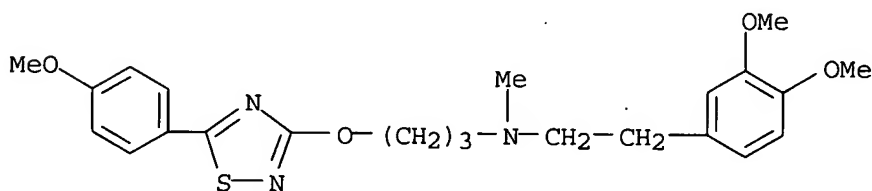
CN Benzenethanamine, N-[3-[[5-(3-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-22-7 HCAPLUS

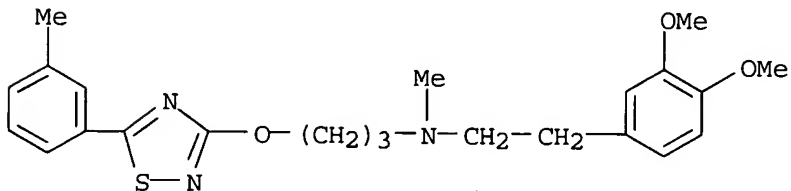
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[[5-(4-methoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-25-0 HCAPLUS

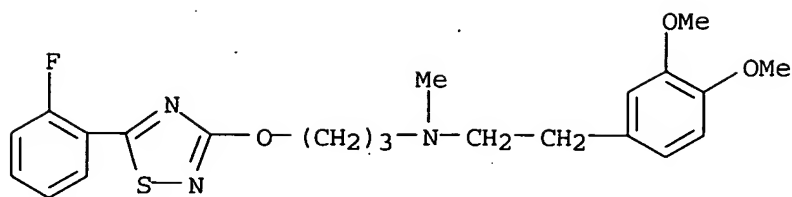
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[[5-(3-methylphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-28-3 HCAPLUS

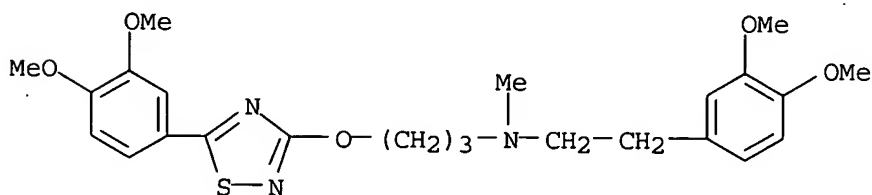
CN Benzeneethanamine, N-[3-[[5-(2-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-34-1 HCAPLUS

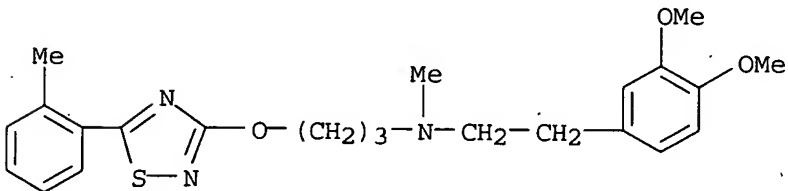
CN Benzeneethanamine, N-[3-[[5-(3,4-dimethoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-39-6 HCAPLUS

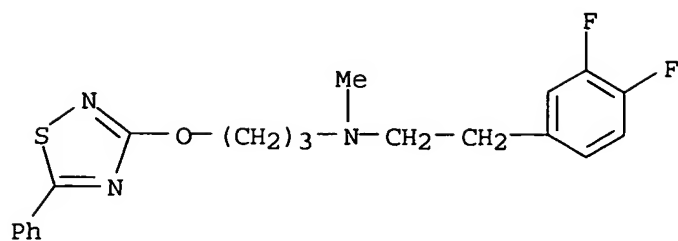
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[[5-(2-methylphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-41-0 HCAPLUS

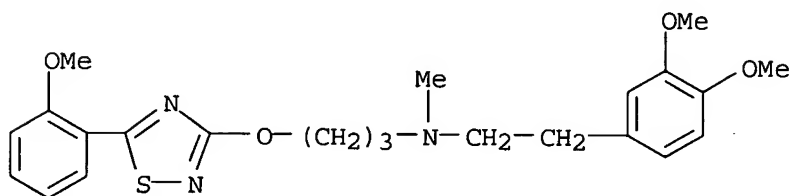
CN Benzeneethanamine, 3,4-difluoro-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-43-2 HCAPLUS

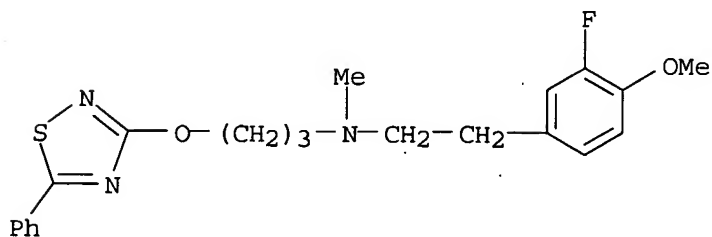
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-45-4 HCAPLUS

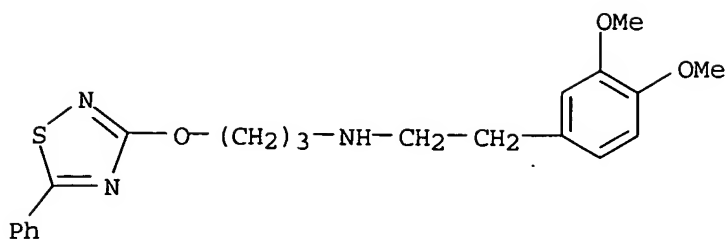
CN Benzeneethanamine, 3-fluoro-4-methoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-50-1 HCAPLUS

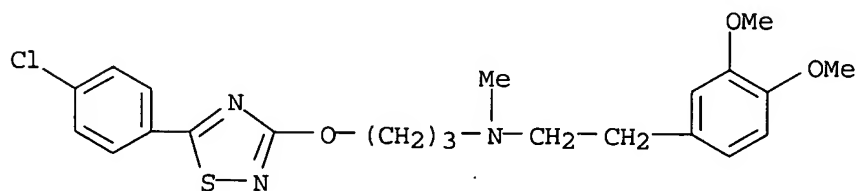
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-57-8 HCAPLUS

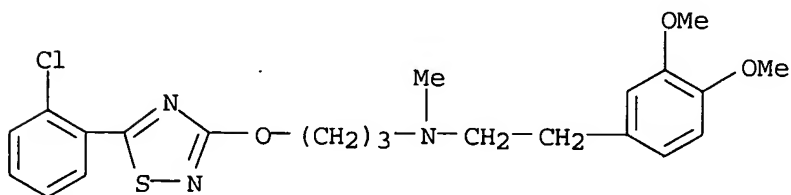
CN Benzeneethanamine, N-[3-[[5-(4-chlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-59-0 HCAPLUS

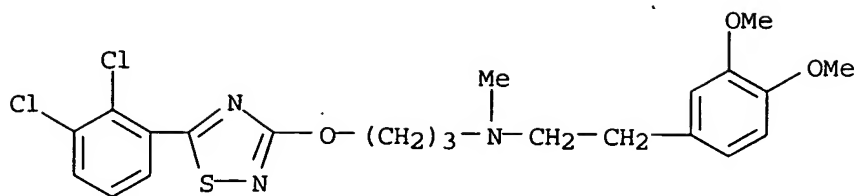
CN Benzeneethanamine, N-[3-[[5-(2-chlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-60-3 HCAPLUS

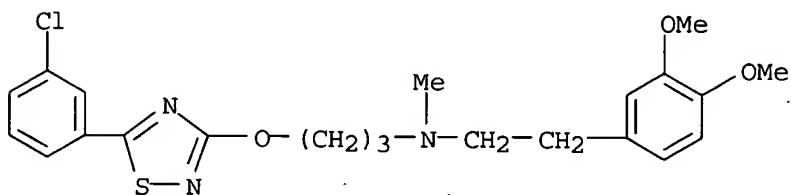
CN Benzeneethanamine, N-[3-[[5-(2,3-dichlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-61-4 HCAPLUS

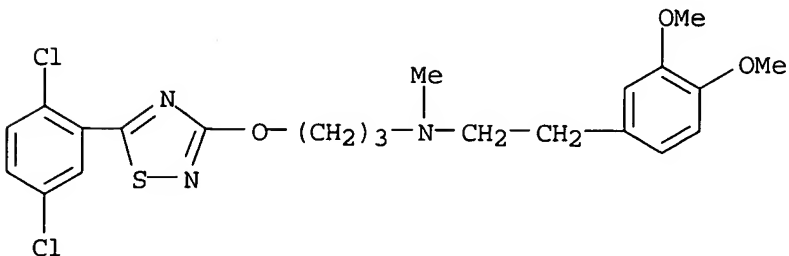
CN Benzeneethanamine, N-[3-[[5-(3-chlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-64-7 HCAPLUS

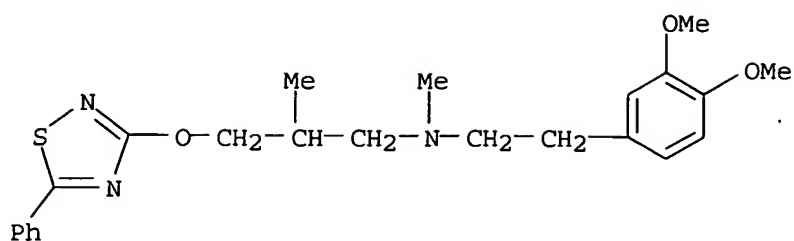
CN Benzeneethanamine, N-[3-[[5-(2,5-dichlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-66-9 HCAPLUS

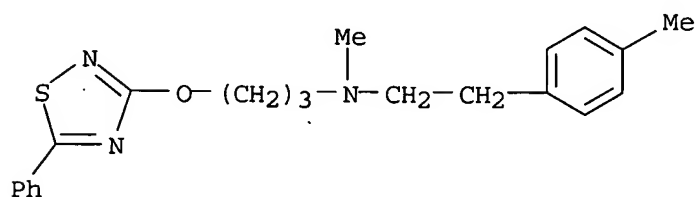
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[2-methyl-3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-71-6 HCAPLUS

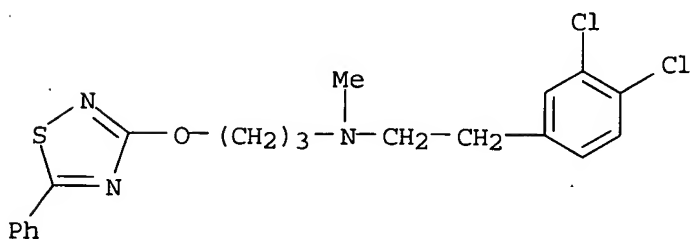
CN Benzeneethanamine, N,4-dimethyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181938-73-8 HCAPLUS

CN Benzeneethanamine, 3,4-dichloro-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

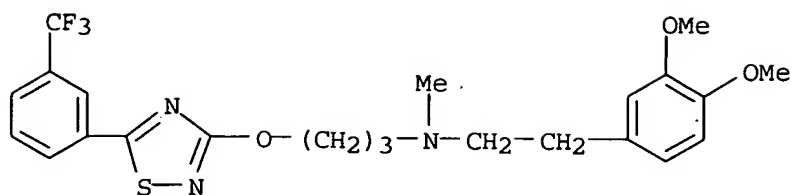


● HCl

RN 181938-75-0 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[[5-[3-(trifluoromethyl)phenyl]-1,2,4-thiadiazol-3-yl]oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

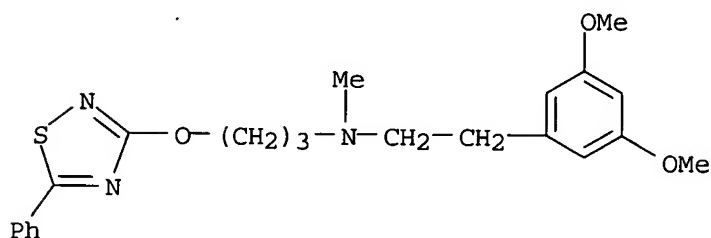




● HCl

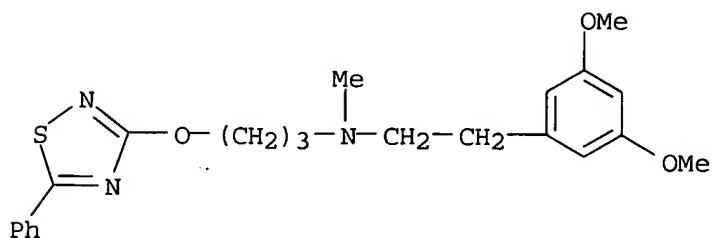
RN 181954-84-7 HCAPLUS

CN Benzeneethanamine, 3,5-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]- (9CI) (CA INDEX NAME)



RN 181954-88-1 HCAPLUS

CN Benzeneethanamine, 3,5-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 181934-76-9P 181935-56-8P 181935-58-0P

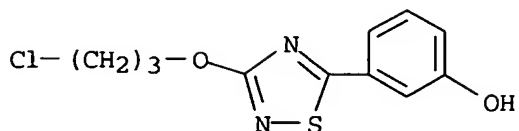
181935-63-7P 181935-71-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

((phenylalkylaminoalkoxy)-heteroaryl compds. having heart-rate-lowering and anti-ischemic effects)

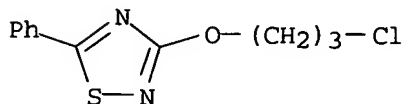
RN 181934-76-9 HCAPLUS

CN Phenol, 3-[3-(3-chloropropoxy)-1,2,4-thiadiazol-5-yl]- (9CI) (CA INDEX NAME)



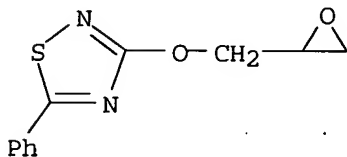
RN 181935-56-8 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(3-chloropropoxy)-5-phenyl- (9CI) (CA INDEX NAME)



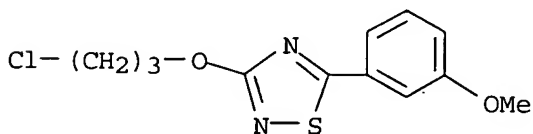
RN 181935-58-0 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(oxiranylmethoxy)-5-phenyl- (9CI) (CA INDEX NAME)



RN 181935-63-7 HCAPLUS

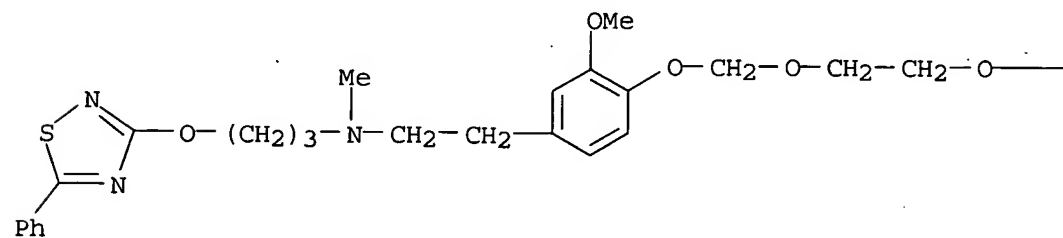
CN 1,2,4-Thiadiazole, 3-(3-chloropropoxy)-5-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 181935-71-7 HCAPLUS

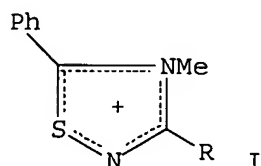
CN Benzeneethanamine, 3-methoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-4-[[2-[(trimethylsilyl)oxy]ethoxy]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



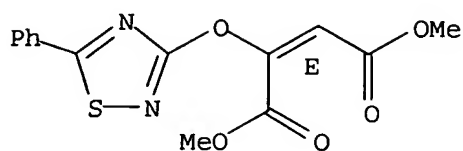
— SiMe<sub>3</sub>

L11 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1984:174732 HCAPLUS  
 DOCUMENT NUMBER: 100:174732  
 TITLE: Cyclic meso-ionic compounds. Part 23. Novel chemistry of 1,2,4-thiadiazoles and their transformation into meso-ionic 1,2,4-thiadiazolium derivatives  
 AUTHOR(S): Newton, Christopher G.; Ollis, W. David; Wright, Derek E.  
 CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, S3 7HT, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (1), 75-84  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 100:174732  
 GI



AB Mesoionic thiadiazolium compds. I (R = O-, N-SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4) were prepared by N-methylation of 3-hydroxy- and 3-(4-toluenesulfonamido)-5-phenyl-1,2,4-thiadiazole, resp. Reactions of 1,2,4-thiadiazoles with nucleophiles follow 2 general paths, reductive transformation to N-thiobenzoyl derivs. and elimination of S with formation of N-benzoyl derivs. A novel route to 1,2,4-thiadiazoles is described in which N-thiobenzoylureas and -guanidines are oxidized by bis(4-methoxyphenyl)telluroxide (II). E.g., treatment of N-methyl-N'-thiobenzoylurea with II in EtOH at room temperature for 30 min gave 84% 2-methyl-5-phenyl-1,2,4-thiadiazole-3(2H)-one.  
 IT 89879-89-0P 89879-90-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 89879-89-0 HCAPLUS  
 CN 2-Butenedioic acid, 2-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]-, dimethyl ester, (E)- (9CI) (CA INDEX NAME)

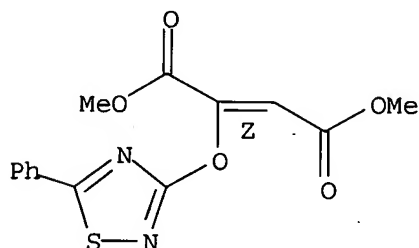
Double bond geometry as shown.



RN 89879-90-3 HCAPLUS

CN 2-Butenedioic acid, 2-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]-, dimethyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

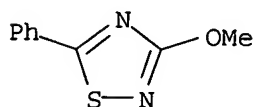


IT 89879-86-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, by methylation of hydroxyphenylthiadiazole)

RN 89879-86-7. HCAPLUS

CN 1,2,4-Thiadiazole, 3-methoxy-5-phenyl- (6CI, 9CI) (CA INDEX NAME)



L11 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:6471 HCAPLUS

DOCUMENT NUMBER: 92:6471

TITLE: Effect of electrophilic reagents on the  
3-hydroxy-1,2,4-thiadiazoles

AUTHOR(S): Taliani, Laurent; Perronnet, Jacques

CORPORATE SOURCE: Cent. Rech., Roussel-Uclaf, Romainville, 93230, Fr.

SOURCE: Journal of Heterocyclic Chemistry (1979),  
16(5), 961-71

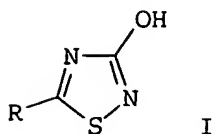
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: French

OTHER SOURCE(S): CASREACT 92:6471

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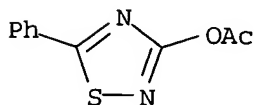


AB Electrophilic reagents may react either with the hydroxyl group in position 3, or with the 2-nitrogen atom of 3-hydroxy-1,2,4-thiadiazoles (I; R = alkoxy, alkylthio, NMe<sub>2</sub>). Hard electrophiles, such as acid chlorides, substitute on OH, whereas soft electrophiles (isocyanates, acid anhydrides) substitute on N.

IT 72183-12-1P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 72183-12-1 HCAPLUS

CN 1,2,4-Thiadiazol-3-ol, 5-phenyl-, acetate (ester) (9CI) (CA INDEX NAME)



L11 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1961:8056 HCAPLUS

DOCUMENT NUMBER: 55:8056

ORIGINAL REFERENCE NO.: 55:1587b-i,1588a-f

TITLE: Thiadiazoles. IX. Reactions of diazonium salts derived from 3-amino-1,2,4-thiadiazoles

AUTHOR(S): Kurzer, Frederick; Taylor, Sheila A.

CORPORATE SOURCE: Univ. London

SOURCE: Journal of the Chemical Society (1960) 3234-9

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 54, 4550a. 3-Halo- and 3-hydroxy-1,2,4-thiadiazoles were synthesized from the corresponding 3-amino compds. by way of the diazonium salts. Of the properties of the new 3-halo-1,2,4-thiadiazoles, their remarkable stability, and the relative inertness of the 3-halo substituent were noteworthy. 3-Amino-5-phenyl-1,2,4-thiadiazole (I) (7.08 g.) in 120 mL. concentrated HCl treated dropwise at -10 to -5° in the presence of a little Cu powder with 5.6 g. NaNO<sub>2</sub> in 15 mL. H<sub>2</sub>O during 45 min., the suspension stirred 15 min. at -8°, 1-1.5 h. at room temperature, and finally 20 min. at 50-60°, diluted with 200 mL. H<sub>2</sub>O, stored at 0°, the crude solid collected, and extracted with ligroine gave residue A. Evaporation of the exts. gave 3.3-4.2 g. 3-chloro-5-phenyl-1,2,4-thiadiazole (II), yellow granules, m. 62-3° (ligroine). II was highly soluble in organic solvents except ligroine. The use of the inverted procedure gave 25% II as did expts. carried out without Cu powder. Residue A (2.5-5.5 g.) was partially fractionated as follows. (a) The residue (2.5 g.) from an experiment extracted at 50° with 30 and 15 mL. N NaOH, the filtered exts. acidified, and the precipitate collected gave 0.65 g. 3-hydroxy-5-phenyl-1,2,4-thiadiazole (III), m. 202-3° (decomposition)

(alc.). (b) The residue (5 g.) extracted with hot H<sub>2</sub>O deposited from the filtrates 1.8 g. solid, which extracted with hot alc. gave 1.1 g. benzoylurea, m. 211-13° (Me<sub>2</sub>CO-alc.). The alc. exts. afforded 0.4 g. III. II resisted hydrogenation at atmospheric pressure in the presence of Raney Ni and PtO<sub>2</sub>. It was unaffected when heated 3 h. at 100° with concentrated H<sub>2</sub>SO<sub>4</sub> but was completely decomposed when refluxed 30 min. in 50% aqueous alc. and M KOH. The compound (70%) was recovered after treatment with MeNH<sub>2</sub>. II was destroyed by N<sub>2</sub>H<sub>4</sub> and failed to react with p-toluenesulfonylhydrazine. II was not convertible into the 3-cyano compound by CuCN. It did not give the 3-thiol on treatment with CS(NH<sub>2</sub>)<sub>2</sub>-KOH (recovery 90%). An intimate mixture of 1.77 g. I and 3.45 g. NaNO<sub>2</sub> was added in small portions during 0.5 h. to 35 mL. 35% HBr at -6 to -8° containing a little Cu powder, the suspension stirred 20 min. at -8°, allowed to reach room temperature during 1.5 h., finally heated at 50-5°, cooled, the mixture added to H<sub>2</sub>O, the oily layer (B) separated, and the aqueous phase extracted with Et<sub>2</sub>O.

The

oily layer B extracted with Et<sub>2</sub>O gave an orange ether solution and an unidentified olive-brown solid. The combined ether exts. evaporated and the residue extracted with ligroine gave a yellow gum. The extract afforded 0.52

g.

3-bromo-5-phenyl-1,2,4-thiadiazole (IV), yellow flakes, m. 64-6.6°. IV was also obtained in 12% yield by the procedure described for II but with 60% HBr. 3-Amino-5-anilino-1,2,4-thiadiazole (IVa) (solvate, 2.38 g.) and 3.45 g. NaNO<sub>2</sub> added during 45 min. to 30 mL. concentrated HCl at -8°, the mixture worked up as described above, the product extracted with 70 mL. hot MeOH, evaporated, and the residue extracted with hot CHCl<sub>3</sub> gave

0.15 g.

5-anilino-3-chloro-1,2,4-thiadiazole, m. 139-41° (50% aqueous alc.). 3-Amino-5-methylamino-1,2,4-thiadiazole p-toluenesulfonate (3.02 g.) in 30 mL. concentrated HCl containing Cu powder treated during 15 min. at -8° with 1.4 g. NaNO<sub>2</sub>, the mixture stirred 51 min. at -8°, at room temperature 0.5 h., and 15 min. at 50-60°, the suspension diluted with 50 mL. H<sub>2</sub>O, and extracted with Et<sub>2</sub>O and CHCl<sub>3</sub> gave 5-7% 3-chloro-5-methylamino-1,2,4-thiadiazole (V), m. 132-4° (H<sub>2</sub>O). V was soluble in H<sub>2</sub>O. A number of attempts made to prepare 3-iodo-5-phenyl-1,2,4-thiadiazole by interaction of the appropriate diazonium salt solution with KI under various conditions were unsuccessful. The yellow liquid obtained on dissolving 1.77 g. I in 10 mL. concentrated H<sub>2</sub>SO<sub>4</sub> treated successively at -8° with 0.76 g. NaNO<sub>2</sub> in 10 mL. concentrated H<sub>2</sub>SO<sub>4</sub> during 10 min. then with 10 mL. 80% H<sub>3</sub>PO<sub>4</sub> during 1 h., 2 g. powdered CO(NH<sub>2</sub>)<sub>2</sub> added during 5 min. and finally 1.7 g. KI in 2 mL. H<sub>2</sub>O-1 mL. 80% H<sub>3</sub>PO<sub>4</sub> during 0.5 h., the mixture stirred 3 h. at room temperature, 100

g.

ice added, the solid collected, washed, the residue dissolved in N NaOH, and the filtered extract acidified gave 0.68 g. III. Basification of the filtrate gave 0.4 g. starting material. II (0.49 g.) in 0.23 g. Na and 5 mL. MeOH refluxed 2 h. gave 0.33 g. 3-methoxy-5-phenyl-1,2,4-thiadiazole, m. 50-1° (ligroine). II (0.0025 mol) heated 1.5 h. with 0.01 g. atom Na in 4 mL. PhCH<sub>2</sub>OH at 80°, the mixture diluted with 0.015 mol 0.5N HCl, the PhCH<sub>2</sub>OH removed, the residual oil extracted with Et<sub>2</sub>O, the solvent removed, and the solid crystallized gave 0.36 g. 3-benzyloxy-5-phenyl-1,2,4-thiadiazole, m. 67-9° (ligroine). II (0.0025 mol) heated during 2 h. with 0.012 g. atom Na in 4 mL. (CH<sub>2</sub>OH)<sub>2</sub>, the mixture stirred into 50 mL. H<sub>2</sub>O, and the solidified oil crystallized gave 0.42 g. 3-(2-hydroxyethoxy)-5-phenyl-1,2,4-thiadiazole, m. 81-2° (ligroine-MeOH). I (1.77 g.) in 15 mL. concentrated H<sub>2</sub>SO<sub>4</sub> and 15 mL. H<sub>2</sub>O diazotized at -10° by adding during 12 min. 1.04 g. NaNO<sub>2</sub> in 4 mL. H<sub>2</sub>O, the mixture stirred a further 15-20 min. at -10°, the temperature raised during 0.5 h. to 25°, the liquid diluted with 25 mL. H<sub>2</sub>O, the suspension heated to 100°, and stored at 0° gave a solid;

the solid dissolved in N NaOH and the solution acidified gave 1.04 g. III. III (0.45 g.) in 8 mL. Ac<sub>2</sub>O refluxed 20 min. gave 0.36 g. mono-Ac derivative, m. 141-2° (alc.). III (0.025 mol) in 5 mL. C<sub>5</sub>H<sub>5</sub>N treated during 15 min. at 100° with 0.7 g. BzCl gave 0.42 g. Bz derivative, yellow prisms, m. 73-5°. III with p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>Cl gave 81% mono-p-toluenesulfonate, needles, m. 93-4° (alc.).

3-Amino-5-(p-nitrophenyl)-1,2,4-thiadiazole (0.55 g.) in 5 mL. concentrated H<sub>2</sub>SO<sub>4</sub> and 5 mL. H<sub>2</sub>O treated at -6 to -8° with 0.26 g. NaNO<sub>2</sub> in 2 mL. H<sub>2</sub>O gave 0.18-0.24 g. 3-hydroxy-5-(p-nitrophenyl)-1,2,4-thiadiazole, orange granules, m. 251-3° (decomposition) (MeOH). Powdered NaNO<sub>2</sub> (1.04 g.) added to 10 mL. cold concentrated H<sub>2</sub>SO<sub>4</sub>, the solution treated during 15

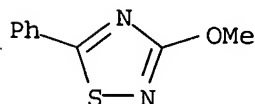
min.

with 2.38 g. IVa in 10 mL. concentrated H<sub>2</sub>SO<sub>4</sub> at -8 to -10°, the mixture stirred while 15 mL. 85% H<sub>3</sub>PO<sub>4</sub> was added during 40 min., the mixture stirred 45 min. at -5°, poured into ice H<sub>2</sub>O, the mixture warmed 10 min. to 50°, filtered, the filtrate adjusted to pH 4, extracted with 80 mL. 40% NaOH, and the filtered solution acidified gave 0.72 g. 5-anilino-3-hydroxy-1,2,4-thiadiazole (VI), m. 207-8° (Me<sub>2</sub>CO-alc.). Acidification of the extract gave a small yield of crude unidentified material, m. between 152-9°. VI (0.5 g.) in 3 mL. POCl<sub>3</sub> refluxed during 0.5 h. and the yellow liquid stirred into ice gave a resinous solid. Addition to the above mixture of 1 mL. PhNMe<sub>2</sub> did not give more favorable results.

IT 89879-86-7, 1,2,4-Thiadiazole, 3-methoxy-5-phenyl-  
99072-03-4, Ethanol, 2-(5-phenyl-1,2,4-thiadiazol-3-yloxy)-  
108619-03-0, 1,2,4-Thiadiazole, 3-(benzyloxy)-5-phenyl-  
(preparation of)

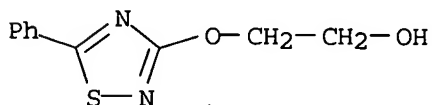
RN 89879-86-7 HCAPLUS

CN 1,2,4-Thiadiazole, 3-methoxy-5-phenyl- (6CI, 9CI) (CA INDEX NAME)



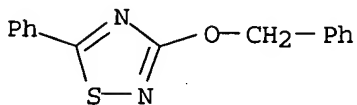
RN 99072-03-4 HCAPLUS

CN Ethanol, 2-(5-phenyl-1,2,4-thiadiazol-3-yloxy)- (6CI) (CA INDEX NAME)



RN 108619-03-0 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(benzyloxy)-5-phenyl- (6CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

135.29

474.44

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-18.00

-18.00

STN INTERNATIONAL LOGOFF AT 08:38:54 ON 05 NOV 2006